Transformation of Europe´s energy-intensive industry sites: A model-based assessment of diffusion dynamics

by Marius Neuwirth

A thesis for the degree of
Doctor technicae

In the
Doctoral Program in Engineering Sciences – Mechanical Engineering

At the
Faculty of Mechanical and Industrial Engineering, TU Wien

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Marius Neuwirth

Abstract

Producing climate neutrally in energy-intensive industries necessitates new and extended infrastructures for hydrogen, CO_2, and electricity. Strategic energy planning requires a high level of spatial resolution, including individual industrial sites. Current models used to evaluate industry transition pathways commonly have limited spatial detail. Combining individual investment decisions with a site-specific spatial resolution contributes to closing the research gap on the spatial and temporal dynamics of industry transition scenarios. In summary, there is a need for spatial high-resolution results to inform decision makers about strategic energy planning, for example, establishing new hydrogen and CO_2 infrastructures.

This thesis focuses on possible diffusion pathways for hydrogen-based industry production with site-specific spatial resolution. Hydrogen-based process options for the energy-intensive industry branches are parameterised to calculate site-specific hydrogen potentials. On that basis, a site-specific open source framework is established to model energy-intensive industries according to their properties. For each existing production unit at the industrial sites, the modelled investment decision among alternative processes is dependent on calculated cost comparisons. Scenario-specific input assumptions influence the cost calculations. The most sensitive parameters for investment decisions in the model are regulations, such as prices for CO_2 certificates, as well as projections of energy prices, and the availability of hydrogen infrastructure. The timing of the investment decision is determined by the age and reinvestment cycles of the production units.

The model is applied to assess transformation pathways dependent on hydrogen infrastructure for the entire large-scale production of primary steel, ammonia, methanol, and high-value chemicals in the EU27+3, analysing 158 plants at 96 sites. Sensitivities are calculated for varying prices of hydrogen and CO_2 certificates, four variations each.

The results show that there is at least one investment window for all plants, while only about one third may have a second investment opportunity before 2050. In addition, more than 30% show reinvestment needs before 2030. Natural gas-based direct reduction of iron ore can play a key role and serve as a bridging option in the transition to the use of green hydrogen for primary steel production. For basic chemicals, especially those where the carbon from fossil feedstocks is embedded within the product, hydrogen prices of 60 €/MWh or below are required for cost-competitiveness of green hydrogen pathways, as carbon prices have only limited effects (scope 1 emissions). The total technical potential for hydrogen use is more than 1000 TWh/yr. Considering current plant ages, reinvestment cycles, infrastructure access, and techno-economic limitations within the 16 sensitivites, hydrogen demand is reduced to 64-507 TWh/yr not considering relocation of value chains.

Kurzfassung

Um klimaneutral zu produzieren, sind neue Infrastrukturen für Wasserstoff und CO_2 sowie ein starker Ausbau für Strom erforderlich. Die strategische Energieplanung erfordert eine hohe räumliche Auflösung, einschließlich einzelner Industriestandorte. Die derzeit verwendeten Modelle zur Bewertung von industriellen Umstellungspfaden verwendet werden, weisen häufig keine ausreichende räumliche Auflösung auf. Die Kombination von einzelnen Investitionsentscheidungen mit einer standortspezifischen räumlichen Auflösung trägt zur Schließung der Forschungslücke in Bezug auf die räumliche und zeitliche Dynamik von industriellen Transformationsszenarien bei. Zusammenfassend besteht daher Bedarf an räumlich hochauflösenden Ergebnissen, um Entscheidungsträger über strategische Energieplanungen, wie den Aufbau neuer Wasserstoff- und CO_2-Infrastrukturen, zu informieren. Diese Dissertation konzentriert sich auf mögliche Diffusionspfade für die wasserstoffbasierte Industrieproduktion mit standortspezifischer räumlicher Auflösung. Wasserstoffbasierte Prozessoptionen für die energieintensiven Industrien werden parametrisiert, um standortscharfe Wasserstoffpotenziale zu berechnen. Auf dieser Basis wird ein standortscharfes Open-Source-Framework entwickelt, um Investitionsentscheidungen in Anlagen von existierenden energieintensiven Industriestandorten anhand ihrer Eigenschaften zu simulieren. Für jede bestehende Produktionseinheit an den Industriestandorten ist die modellierte Investitionsentscheidung zwischen alternativen Prozessen abhängig von der berechneten Wirtschaftlichkeit. Die Kostenberechnung wird durch szenariospezifische Input-Annahmen beeinflusst, wie z. B. Energiepreisentwicklungen, Regulierungen wie Preise für CO_2 Zertifikate und die Verfügbarkeit von Wasserstoffinfrastruktur. Der Zeitpunkt der Investitionsentscheidung wird wird durch das Alter und die Reinvestitionszyklen der Produktionseinheiten bestimmt.
Mit Hilfe des Modells werden Transformationspfade für 158 Anlagen an 96 Standorten für die gesamte großtechnische Produktion von Primärstahl, Ammoniak, Methanol und Plattformchemikalien in der EU27+3 bewertet. Unterschiedliche Preisannahmen für Wasserstoff und CO_2-Zertifikate führen zur Berechnung von 16 Sensitivitäten. Die Ergebnisse zeigen, dass alle Anlagen ein Investitionsfenster bis 2050 haben, aber nur ein Drittel eine zweite Möglichkeit. Über 30% zeigen einen Reinvestitionsbedarf vor 2030. Die erdgasbasierte Direktreduktion kann eine Schlüsselrolle spielen und als Brückentechnologie der Stahlproduktion hin zur Nutzung von grünem Wasserstoff dienen. Die CO_2-Preise (auf Scope 1 Emissionen) zeigen bei einigen Grundstoffchemikalien nur begrenzte Wirkung, da Teile des Kohlenstoffs im Produkt gebunden sind. Wasserstoffpreise unter 60 €/MWh sind daher zur Wettbewerbsfähigkeit erforderlich. Die berechneten Sensitivitäten ergeben eine Wasserstoffnachfrage von 64-507 TWh in 2050 bei einem technischen Potenzial von über 1000 TWh. Eine Verlagerung von Wertschöpfungsketten ist dabei nicht berücksichtigt.

Acknowledgements

After five years of studying at the Karlsruhe Institute of Technology (KIT), I started my Master's thesis as a cooperation at the TU Wien. At that time, the intention and goal of writing a dissertation was still far away. Back in Karlsruhe, I got the opportunity to join Fraunhofer ISI, where I wanted to contribute to projects aiming at defossilising the industry. Early in this stage within the new field, I felt that research could benefit from higher spatial resolution in industry modelling and the representation of single sites.

I am, of course, grateful to the people who made this dissertation possible. First and foremost, my supervisor Prof. René Hofmann, who openly received my "Exposé" and supported me in further detailing the topic. At the same time, my supervisors and mentors at the Fraunhofer ISI, Tobias Fleiter and Martin Wietschel, laid the foundation with their support and trust to complete this project.

I also thank all the colleagues from whom I have learnt a lot, who have encouraged me and who have helped me through some tough times with their expertise and humour. I would especially like to thank the colleagues in my business unit *Demand Analyses and Projections* - Andrea, Khaled, Matthias, Pia, Thurid, Stefan, Sirin, Simon, Luna. Thank you all for your positiveness and helpfulness.

My family, of course! Without your incredible support I could never have taken the path I did. In particular, my dad Manfred, who sadly passed away in 2019, and my mum Monika have always been and continue to be my most important mentors, fans, and supporters. I am especially grateful to my brother Matthias for his role model function. From you, I have adopted a lot regarding determination and independence.

Lastly, I thank my girlfriend Natalia. Understanding, loving, and humorous, you always managed to calm me down and give me the necessary distance from this dissertation project. You helped me to prioritise this work correctly on the list of life's priorities and regain creativity with the necessary serenity. You continually show me why our life is so valuable and what really matters to both of us. I love looking into the near future, getting parents soon, and starting a new phase of life.

The greatest threat to our planet is
the belief that someone else will save it.

ROBERT SWAN

Preface

This cumulative dissertation was composed at the TU Wien at the Institute of Energy Systems and Thermodynamics[1] during my employment at the Fraunhofer Institute for Systems- & Innovation Research (ISI)[2]. The integration in project work at Fraunhofer ISI led to contributions in numerous research projects. Some of these projects thankfully had synergies with this PhD topic and are thus strongly connected with the publications and content within this dissertation.

Three published journal articles build the core publications of this thesis, complemented by five peer-reviewed conference contributions - two as the main author and three as a co-author. An extensive list of projects and reports can be found at the end. In the following a selection of the most contributing projects is given, to which also the core publications of this thesis refer.

- ***TransHyDE-Sys***; BMBF - research project; Grant number: 03HY201L; https://www.transhyde.de/
- ***TRANSIENCE***, European Commission, Horizon Europe project; Grant number: 101137606.
  https://www.transience.eu/
- ***Langfristszenarien III***; BMWK; Grant number: 03MAP392
  https://langfristszenarien.de
- ***Ariadne & Ariadne 2***; BMBF - research project; Grant number: 03SFK5D0 & 03SFK5D0-2;
  https://ariadneprojekt.de/
- ***sEEnergies***; European Commission, Horizon 2020 project; Grant number: 846463.
  https://www.seenergies.eu/
- ***VerSEAS***; BMBF - research project; Grant number: 03EI1018C.

Within the Fraunhofer CINES (Cluster of Excellence Integrated Energy Systems) some of the work necessary to conduct this thesis, complemented with fruitful discussions, was supported.

[1] https://www.tuwien.at/en/mwbw/iet/e302-03-research-unit-of-industrial-energy-systems
[2] https://www.isi.fraunhofer.de/en/competence-center/energietechnologien-energiesysteme/geschaeftsfelder/nachfrageanalysen-projektionen.html

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Nomenclature

Acronyms

AGEB	German Working Group for Energy Balances
ARRRA	Antwerp-Rotterdam-Rhine-Ruhr Area
CCUS	Carbon Capture, Utilisation, and Storage
CO_2	Carbon Dioxide
DRI	Direct Reduced Iron
EAF	Electric Arc Furnace
ECEMF	European Climate and Energy Modelling Forum
EHB	European Hydrogen Backbone
ESM	Energy System Model
EU	European Union
GHG	Greenhouse Gas
H_2	Hydrogen
H2-DRI	Direct Reduced Iron using Hydrogen
HT	High Temperature
HVC	High Value Chemicals
IAM	Integrated Assessment Model
IPCC	Intergovernmental Panel on Climate Change
LT	Low Temperature
LULUCF	Land Use, Land Use-Change and Forestry

NG	Natural Gas
NG-DRI	Direct Reduced Iron using Natural Gas
NUTS	Nomenclature des Unités Territoriales Statistiques
RED	Renewable Energy Directive
RES	Renewable Energy Sources
RFNBO	Renewable Fuels of Non-biogenic Origin
RQ	Research Question
SAF	Sustainable Aviation Fuels
SEC	Specific Energy Consumption
SHC	Specific Hydrogen Consumption
SMR	Steam Methane Reforming
SSM	Sector-Specific Model
TRL	Technology Readiness Level
TWh	Terawatthours ($3.6 \cdot 10^{15}$J)
TWh/yr	Terawatthours per Year (($3.6 \cdot 10^{15}$J)/yr)
°C	Temperature in Degree Celsius

Research summary

This research summary highlights the identified research gaps, presents the context in current research, and connects the core publications to outline the closed gaps through the continuous progress in this dissertation.

The Introduction emphasises anthropogenic climate change as one of the biggest challenges in the world. Mitigation of greenhouse gases (GHG), especially carbon dioxide (CO_2) emitted for energy purposes, is necessary to combat climate change. A major part of global and European GHG emissions results from industrial processes. Thus, the present thesis investigates on modelling the transformation of the industry sector towards climate-neutral production.

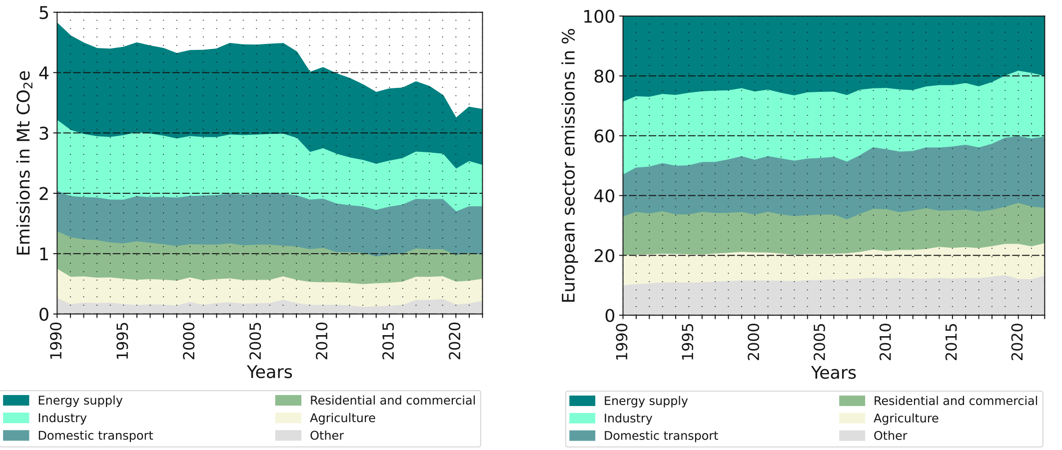
The scientific knowledge on industry decarbonisation options and methodological state-of-the-art of industry transition models before the beginning of this thesis is outlined in section 2. The research questions and the scope of the industry model developed are highlighted and placed in section 3. The identified research gap that is addressed in the *Key objective*, which is structured into three research questions. The research questions RQ 1 to RQ 3 and subquestions are answered by a series of scientific publications. The individual publications and results are summarised and put into context in section 4. The key findings of the publications are summarised in section 5.

In section 6 conclusions are drawn from the publications and their relation to the topic of the dissertation and the scientific contribution is discussed. Finally, the limitations of the entire work are highlighted within a critical assessment and an outlook for possible future research is given.

1 Introduction

> *"Warming from anthropogenic emissions from the preindustrial period to the present will persist for centuries to millennia and will continue to cause further long-term changes in the climate system [...], but these emissions alone are unlikely to cause a global warming of 1.5°C [...]. Human activities are estimated to have caused approximately 1.0°C of global warming above preindustrial levels, with a likely range of 0.8°C to 1.2°C. Global warming is likely to reach 1.5°C between 2030 and 2052 if it continues to increase at the current rate".* - Intergovernmental Panel on Climate Change 2018

Global climate change is one of the biggest challenges of the 21st century, and emission reduction is indispensable to mitigate global warming and its disastrous consequences. As part of the *"Paris Agreement"*, the signatory nations, including the entire European Union (EU), agreed to limit global warming to well below 2 °C, preferably even 1.5 °C (United Nations Framework Convention on Climate Change 2015).
The EU adopted emission reduction targets proposed by the European Commission with its *"Fit-for-55-Package"* of 55% in 2030 compared to 1990 (European Commission 2021), while climate neutrality should be reached according to the *"European Green Deal"* by 2050 (European Commission 2019). Figure 1 shows the development of GHG emissions in the EU from the energy supply and demand sectors (Fig. 1a) and their sector-specific shares (Fig. 1b). The demand sectors can be classified into domestic transport, residential and commercial services, agriculture, industry and others (containing international bunkers, waste, land use, land-use change and forestry (LULUCF), and other combustion) (European Environment Agency 2024).



(a) *Development of total European GHG emissions from 1990 to 2022*

(b) *Development of sectoral emission shares from 1990 to 2022*

Figure 1: *Overview of the development of GHG emissions in the EU from 1990 to 2022 (Source: own figure with data from European Environment Agency 2024)*

A successful energy transition requires both the expansion of renewable energy sources (RES) to decarbonise the energy supply sector and the improvement of energy efficiency, as well as a fuel switch in the demand sectors (International Energy Agency 2024). Especially energy-intensive industries contribute largely to industrial GHG emissions, such as steel and basic chemicals, and pose a particular challenge in achieving European climate targets. Figure 1 illustrates that with 20% in 2022, the industrial sector was a major contributor to the total GHG emissions (European Environment Agency 2024). In addition, European industries are dependent on fossil fuels and consume nearly 30% of the final energy use in the EU (Eurostat 2022). Consequently, significant efforts are needed to replace fossil fuels in various processes. The i) direct use of renewable electricity and ii) synthetic energy carriers derived from renewable sources, together with iii) carbon capture utilisation and storage options, or iv) biogenic energy carriers, can play an important role in industrial decarbonisation (Möst et al. 2020).

Around 1800 TWh of fossil fuels, mainly natural gas and oil products, were used in the EU27 in 2022 (Eurostat 2022). Process heat applications usually depend on natural gas, while chemical production relies on natural gas and oil products as feedstocks. Natural gas for process heat can be replaced in many applications by retrofitting burners and process configurations for climate-neutral molecular energy carriers, such as hydrogen, while direct electrification of process heat applications shows advantages in energy efficiency (Thiel & Stark 2021; Fleiter et al. 2024b). However, switching to direct electrification requires more fundamental changes, such as new steam generators or furnaces. Additionally, direct electrification for high-temperature (HT) processes technical maturity may not be sufficient for high-temperature (HT) processes according to current research (Fleiter et al. 2024b). In summary, the potential for direct electrification of industrial process heat is enormous, while technical, economic, and organisational barriers, such as the expansion of the connected power input of industrial sites, still exist (Thiel & Stark 2021; Rehfeldt et al. 2024). These uncertainties, especially for HT processes, and the need to replace fossils in feedstock applications highlight the need for climate-neutral molecular energy sources, either synthetic or biogenic. From a systemic perspective, the energy demand mix can diverge drastically depending on the decision for direct electrification or other molecular-based process options, which extends uncertainties to the energy supply. In addition, uncertainty in the timing of investment decisions adds another layer of complexity to the transformation of the industrial sector. Consequently, developments in the energy transition on both the demand and supply side highly affect the development of energy infrastructures and therefore need to be assessed (Kamali Saraji & Streimikiene 2023; Hassan et al. 2024).

Hydrogen can be used in various industrial processes for energetic and feedstock applications and provides the basis for all synthetic energy carriers. Produced from renewable electricity via electrolysis, it offers a promising solution towards climate neutrality (Neugebauer 2023). Moreover, hydrogen and a variety of its derivatives offer significant benefits where direct electrification shows weaknesses: they enable long-term storage to balance fluctuations in RES and provide flexibility for energy and feedstock applications (Usman 2022; Muhammed et al. 2022; Tackie-Otoo & Haq 2024; Fleiter et al. 2024a). The transportability of these molecular hydrogen derivatives can help address regional supply and demand discrepancies, but requires appropriate infrastructure for storage and transportation (Fleiter et al. 2024a). In addition, also intra- and intercontinental long-term energy transport is possible.

With the REPowerEU plans, the European Commission is pursuing efforts to establish a green hydrogen economy (European Commission 2022a). This legislation aims at a total of 20 megatonnes of hydrogen use in the EU in 2030, of which 10 megatonnes should be produced domestically and 10 megatonnes imported (European Commission 2022a). Nevertheless, currently hydrogen plays only a role in the petrochemical industries, predominantly produced from natural gas (Dechema 2017). Despite legislation tries to push for a green hydrogen economy, industries still use grey hydrogen instead of green hydrogen. This indicates one of the main problems in the transition of the industry sector: Currently, fossil fuels are still available at low prices compared to renewable energy carriers.

Established subsidies for fossil energy sources and missing policies supporting renewable energy carriers lead to lock-ins through new investments in fossil-based industrial processes. These investments, in turn, lead to a sustained demand for fossil fuels, which stimulates their continued supply. Thus, the future economic competitiveness of energy carriers based on renewable energy sources compared to fossil fuels is uncertain, while GHG emissions must decrease faster than observed in the past (Fig. 1) to meet the goals for GHG neutrality. Implementing climate-neutral industry processes may require access to newly constructed pipelines or a reasonable expansion of the capacity of the electricity grid. Strategic planning of such infrastructures requires robust analyses of the spatial and timely development of energy demand for the respective energy carriers. Current approaches in the context of energy system analysis for modelling the energy transition still lack spatial resolution and knowledge about the spatial and temporal transition dynamics. In addition, the transition to renewable energy systems is a complex task, hindered by specific barriers such as technological limitations, high initial costs, regulatory challenges, and the need for infrastructure upgrades. Four of the main barriers for energy-intensive industries to switch to climate-neutral production are raised in literature by Wesseling et al. 2017:

- **Huge investments** in new processes or changes in current process designs.
- **Lack of guaranteed availability** of renewable energy carriers.
- **Technological maturity** of new processes that have not yet been demonstrated.
- **Price uncertainties** of sustainable energy carriers lead to unclear economic viability.

In summary, lock-in effects with reliance on fossil fuels are generated due to a lack of viable and economic climate-neutral alternatives. To break through these mechanisms and enable the diffusion of climate-neutral industrial processes, strategic systemic decisions for a sustainable transformation are inevitable. One of the most crucial systemic decisions is the expansion of the electricity grid and the infrastructure ramp-up for green energy carriers, such as hydrogen. The topology of new infrastructure and the allocation of necessary grid expansion require robust analyses on the spatial distribution as well as on the timely diffusion pathways. Therefore, considering regional and temporal developments is essential to gain knowledge about future spatial and temporal dynamics to assess reliable pathways for industry transition.

The investigation of spatial and temporal dynamics in industry transformation motivates this thesis. The direct electrification of industrial process heat can have energy efficiency and economic advantages compared to hydrogen if the technology is technically mature (Sorknæs et al. 2022). However, the use of hydrogen as a reducing agent for direct reduction (H2-DRI) in steel production and as feedstock in basic chemicals is considered promising and has no renewable alternatives for green production processes projected to be mature until 2050. Therefore this thesis focuses on the methodological development to improve the spatial and timely representation of industrial diffusion dynamics applied for hydrogen-based production of primary steel, ammonia, methanol, and high value chemicals (HVC).

2 Context

The transition to a climate-neutral industry relies on renewable energy sources. The introductory section 1 gives a brief overview of the challenges related to climate change, the political landscape, and its actions to achieve the emission mitigation targets. Hydrogen is a promising option for energy-intensive industries and requires reliable infrastructure (Fleiter et al. 2024a). Therefore, analyses for spatial and temporal dynamics in a systemic context need to become more robust and detailed.

2.1 Modelling tools for climate and energy system research

The findings of the 1.5°C IPCC report (Intergovernmental Panel on Climate Change 2018) are the basis for the Paris Agreement, as well as for national and international political targets. This IPCC report is the result of scientific predictions based on a variety of potential future pathways derived from several modelling tools. Modelling tools have become increasingly important in recent decades in order to gain insight into the complex connections and dependencies between the individual components of the energy system. Müller et al. 2018 present an overview of the modelling tools used in Europe within the European Climate & Energy Modelling Forum (ECEMF) on integrated assessment, energy system and sector-specific resolution. Many of them are distinguished by top-down, bottom-up, and hybrid approaches by Prina et al. 2020. Top-down models usually show a simplified representation of the energy system and focus on macro- and socio-economic indicators to understand the broad economic impacts of energy policies. The bottom-up modelling approaches are usually not able to capture macro- and socio-economic effects but emphasise the techno-economic characteristics and cost-competitiveness of individual technologies and processes. Hybrid approaches try to combine both approaches by integrating sectoral bottom-up results into macro- and socio-economic top-down approaches. Integrated assessment models (IAMs) often represent such hybrid approaches that work with detailed results of the energy system and specific sectors to investigate broad macro- and socio-economic consequences.

Integrated assessment models (IAMs) quantify various systems and abstract the reality to provide information on future developments of the covered systems. IAMs aim to unify the social, environmental, economic, political, and regulatory aspects and their interactions in a holistic approach to obtain robust predictions on the resulting implications. To investigate different possible future paths, assumptions and long-term projections about the economy, environment, society, and technologies are necessary (Braunreiter et al. 2021). Their most common use is related to climate change mitigation (Dowlatabadi 1995; Braunreiter et al. 2021). These models often incorporate different spatial trends and developments based on a breakdown to several regions and merge the results to draw conclusions at a global level. Dowlatabadi 1995 provides an overview over early integrated assessment approaches, representing phase 1 and phase 2 in the classification of van Beek et al. 2020 to categorise the rise of IAMs over the last decades. Nikas et al. 2019 reviewed a number of 60 IAMs and classified them by means of their methodological approach. Confirmed with other reviews in the literature, most of the early models are still dominating the field of IAMs, i.e. MARKAL/TIMES (Loulou & Labriet 2008; Loulou 2008), REMIND (Luderer et al. 2013), $\text{MESSAGE}_{\text{ix}}$ (Huppmann et al. 2019). However, they are meanwhile complemented by numerous others, such as MEDEAS (Nieto et al. 2020) and MUSE (Giarola et al. 2022). Development and comparison of such a variety of different models enables to derive robust conclusions from their results and to identify uncertainties on future projections. IAMs help to understand the impacts of human behaviour by analysing multiple possible scenario developments. Therefore, strong assumptions are necessary on a broad variety of variables for sectoral developments in a very aggregated manner. International institutions like the IPCC use the results to analyse the scenarios and to carve out risks and necessary courses of action to prevent against social and environmental catastrophes. In this regard, IAMs provide policy-relevant insights and evaluate different policy strategies regarding their achievements and consequences.

The briefly described IAMs are based on various inputs. Due to the global and broad sectoral scope they use results derived by much more detailed energy system models (ESMs). According to the classification of Nikas et al. 2019, ESMs focus on the energy sector and are a subcategory of partial equilibrium IAMs. Improvements by those models have multiple dimensions, e.g. time-, spatial-, and technological resolution.

Energy system models (ESMs) are tools designed to analyse the dynamics within an energy system, encompassing the production, conversion, distribution, and consumption of energy. These models assess the impact of energy policies, technological progress, and investment strategies under various future scenarios (Pfenninger et al. 2014; Connolly et al. 2010). Moreover, ESMs help to explore the potential pathways towards sustainable and low-carbon energy systems. They help identify the optimal mix of energy technologies and practices that can meet future energy demands while minimising environmental impacts (Bhattacharyya & Timilsina 2010). As for IAMs, also the role of ESMs in strategic energy planning and policy-making becomes increasingly important, guiding decisions that balance economic, environmental, and social objectives. ESMs show a diverse field of application with individual scopes and methods, making it difficult to group them. Approaches range from simple frameworks with broad assumptions to complex integrated models. Connolly et al. 2010 reviewed 68 existing modelling tools and clustered 37 of them by various indicators, such as covered energy sectors or geographical areas. Examples for ESMs that are well-known in European energy contexts are especially PRIMES (E3Modelling 2018), as well as Enertile, SCOPE SD and REMod (Schmitz et al. 2024), PyPSA (Hörsch et al. 2018; Brown et al. 2018; Brown et al. 2023), REMix (Gils et al. 2021; Wetzel et al. 2023) and energy system modules within the frameworks already named under the IAMs section. A more comprehensive list and their individual model characteristics are given by Herbst et al. 2012, Ringkjøb et al. 2018, Müller et al. 2018, and Prina et al. 2020. Fodstad et al. 2022 analysed the challenges that current ESMs face in timely, regional, political, and technological dimensions and applied them to the existing ESMs mentioned above for the European context.

ESMs sometimes have integrated submodules for energy supply, conversion, and infrastructure, as well as energy demand, which represent individual sectors at a fairly high level of aggregation. Especially infrastructures are often investigated without considering detailed site-specific spatial attributes, but rather on a more aggregated spatial resolution by general conclusions on the monetary factors of the optimised energy system (Gils et al. 2021; Neumann et al. 2023).

However, some ESMs also integrate results from detailed sector-specific models (SSMs) as exogenous input, allowing for a nuanced understanding of the components of the energy system. Consequently, IAMs make use of ESMs, which themselves build on or exist of SSMs.

Sector-specific models (SSMs) are used to understand and predict the dynamics within specific sectors. In the context of integrated assessments and energy system analysis, SSMs are crucial for examining the nuances of energy supply and conversion, distribution and infrastructure, as well as energy consumption within different sectors such as industry, transport, households, and others. Several models exist for the various sectors. Examples for the energy demand sectors in Europe are ALADIN (Gnann & Plötz 2015; Cao Van et al. 2023) for the transport sector, ATOM (Stavrakas et al. 2019) for the residential sector, DREEM (Stavrakas & Flamos 2020) for buildings, FORECAST (Fleiter et al. 2018), WISEE-EDM (Bilici et al. 2024) and IndustryPLAN (Mathiesen et al. 2023) for the industry sector. There are various other studies and models, without giving the models dedicated names. Reviews and an overview on those can be found in literature for the transport (Gnann et al. 2018), residential (Moglia et al. 2017), and other sectors. These models investigate on the detailed aspects of their respective sectors by incorporating sector-specific data. They can simulate the effects of technological changes, such as the adoption of renewable energy technologies, improvements in energy efficiency, and the effect of policy interventions such as carbon pricing or different subsidies (Suganthi & Samuel 2012). SSMs often focus on prediction and market diffusion patterns to evaluate regulations and provide an analysis of trends, challenges, and policy impacts. The adaptation of new data, technological developments, and sectoral challenges is an essential part of the continuous development of SSMs. The integration of sector models within broader system models can provide a more comprehensive understanding, enabling stakeholders to make informed decisions that consider interdependencies among sectors. Industry sector models often assess the potential for energy efficiency improvements the implementation and diffusion of new processes. Industry sector models typically assess the turnover of the existing plant stock with high technological resolution based on techno-economic behaviours and environmental challenges. Assessments of possible future pathways by switching to climate-neutral energy carriers and reduction of sectoral carbon footprint are purposes of industry models.

In summary, IAMs, ESMs, and SSMs have evolved greatly over the last decades and are meanwhile powerful tools for future projections and policy guiding. Therefore, a tentative and transparent interpretation of the underlying assumptions and the respective model results is crucial. Critical reviews can be found on topics like modelers' assumptions and influences (Ellenbeck & Lilliestam 2019), recognition of justice principles (Rubiano Rivadeneira & Carton 2022) as well as insufficiency in unpredictable social crises (Koasidis et al. 2023) and political (van Beek et al. 2022) or general (Schwanitz 2013) evaluations. Those reviews help in interpreting the different models and in drawing conclusions on general trends and behavioural changes. However, IAMs are highly dependent on reliable inputs and assumptions while abstracting reality. Input data for energy system aspects in IAMs are often provided by ESMs, which have a more detailed focus on optimisation of energy supply, conversion, distribution, and consumption with a better spatial and timely resolution. As these ESMs focus on the supply and distribution of the energy system, they rely on the results of detailed sector investigations by SSMs.

2.2 Scope and methods of modelling tools

The models reviewed in section 2.1 have different scopes and methods to address a wide range of research questions. In general, there are many models that address different perspectives with different resolutions on both regional and sectoral granularity. Some focus on different corners of the energy system, while others optimise the whole system on different regional levels with simplified assumptions on individual aspects. The energy transition requires highly resolved results in the different dimensions to guide a collective approach in which stakeholders can act with coordinated planning according to political guidelines to support investment decisions. Prina et al. 2020 characterised the various bottom-up models for energy system analysis according to five classifications: covered energy sectors, geographical coverage, time resolution, underlying methodology, and programming technique. As a result, short-term bottom-up models more often use a simulation approach, whereas long-term bottom-up models are predominantly based on optimisations. While especially IAMs and ESMs often rely on optimisation approaches with relatively low spatial resolution, sector models may operate more realistically when implemented as simulations to capture different behaviours. An optimisation of only one sector would be a very local optimum, which is not appropriate to integrate in energy system analysis. Overall, both optimisation and simulation methods are legitimately used for various questions, and the differences are briefly described in the following.

Optimisation models solve an arbitrarily complex system of equations depending on the question at hand. These methods are used to minimise or maximise a specific parameter or to achieve a balance between different variables. Constraints are specified within which an optimal solution is to be found. A broad variety of optimisation techniques exists, which all have their advantages depending on the problem to be resolved, and help in decision-making under uncertainty.

In the context of energy system analysis, optimisation approaches are typically used for the energy supply sector. Here, exemplary optimisation problems are minimising costs, maximising energy output, or balancing both to achieve the most economical implementation and diffusion of renewable energies to achieve political climate goals. Constraints enable more realistic assumptions by setting limits or requirements to be met for certain parameters of the optimisation problem. Examples include environmental regulations and resource availability, as well as regional potentials for renewable energy, political targets for the expansion of renewable energy, or the availability of technologies. Finally, such optimisation approaches can support the planning of energy systems by providing insights into the improvement and reliability of energy supply and the integration of renewable energy.

Simulation models, on the other hand, are not intended to find optimal solutions to problems. The purpose of simulation models is to provide a near-to-reality representation and possible future developments of a system, depending on varying assumptions and framework conditions. In the context of energy system analysis, the goal is to estimate various behaviours and reactions to external developments in scenario analyses to identify potential issues and to evaluate the impact of different strategies. Those simulation models are highly dependent on their input data. Some of the exogenous input data for future projections is necessarily based on exogenous assumptions.
Simulation approaches help to develop strategies and inform stakeholders to anticipate future challenges. This information supports the evaluation of resilience and sustainability in energy systems. These models can demonstrate potential future developments in various scenarios. The scenario results assist in developing more robust energy policies and systems. These simulation methods enable to integrate more individual decision-making and provide detailed insights into system behaviours, to enable more informed and effective energy and policy planning.

Orientated at the definitions of Prina et al. 2020, Figure 2 shows the scope and resolution of the approach of this work in the context of climate and energy system research.

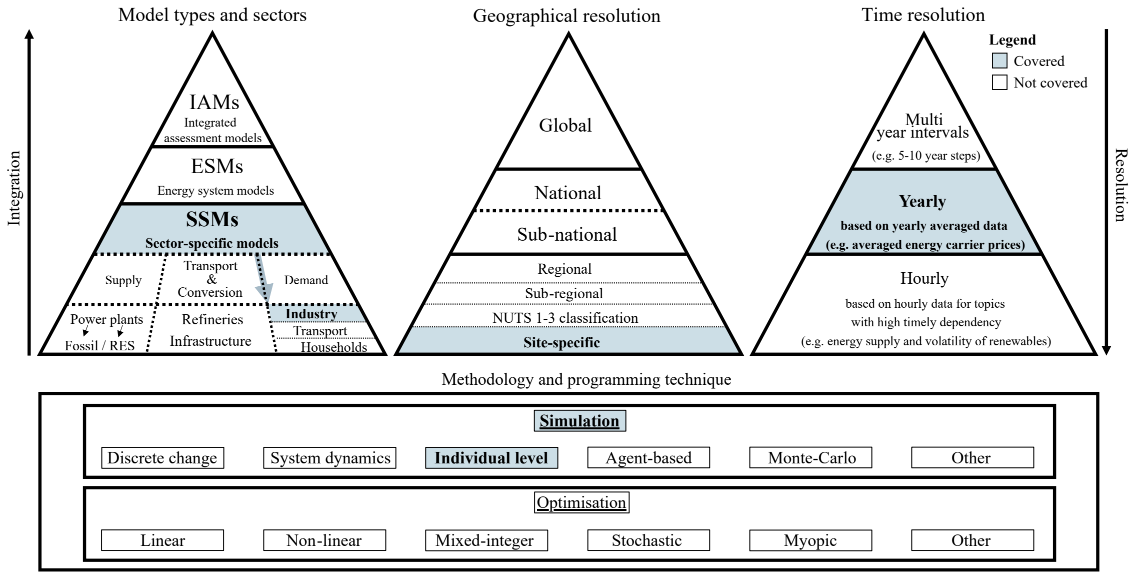


Figure 2: *Placement of the developed modelling approach within the field of climate and energy system research.*

The decision to use a simulation approach in this dissertation is based on the differences between optimisation and simulation, as well as the mathematical distinction between direct and indirect problems. Direct problems are characterised by known input data, and the corresponding output data can be determined. In contrast, the objective in indirect problems is to identify the path to reach a specific output. Thus, ESMs are often formulated as indirect problems, typically relying on optimisation techniques. The target function, such as minimising system costs while achieving climate neutrality by 2050, is predefined in order to find the most cost-effective path under the respective boundary conditions. On the other hand, SSMs mostly represent direct problems. These models focus on understanding reactions and developments within a sector to exogenously given conditions, such as energy price projections, starting from a known initial state. This observation is justifiable when analysing other industry sector approaches. Industry sector models, or industry representations within IAMs and ESMs, are predominantly based on simulation approaches, as data availability is scarce and future developments are uncertain (Edelenbosch et al. 2017). Consequently, some drivers for industry transition patterns are hard to cover by endogenous modelling, leading to difficult constraint definition in optimisations, which makes it more reasonable to build on a simulation approach with exogenous assumptions. As already listed in chapter 1, uncertainties in investment decisions and future projections are the result of unclear economic competitiveness due to missing policy guidance in the past.

In addition, two aspects are substantial to conduct reliable analysis from a system perspective, especially when it comes to the need for alternative energy carriers and infrastructure requirements. First, to identify bottlenecks between the industry sector, energy infrastructure, and energy supply, high spatial resolution is necessary. Although some models already show improved geographical coverage by using multi-node approaches, none could be found in the literature that offer site-specific resolution (Fodstad et al. 2022). Second, the temporal dynamics and the market diffusion of new processes need to be connected to the spatial component to support strategic and systemic decision making. The age structure of individual plants and their reinvestment cycles determine the diffusion speed of new processes and the belonging change in energy demand (Wesseling et al. 2017). The following sections 2.3 to 2.5 further elaborate on the current implementations of diffusion behaviour in ESMs and demand models such as SSMs. Section 2.6 investigates the challenges of industry sector modelling and reviews the best-known current implementations and approaches.

2.3 Adoption patterns in diffusion theories and models

Technology diffusion describes the diffusion process as the spread of an innovation over time (Stoneman & Battisti 2010). Many theories attempt to describe the various influencing factors to predict the degree of dissemination and the underlying decision-making processes. Rogers' theory of the diffusion of innovations forms the basis for adoption patterns in various application areas and adapting dissemination strategies (Rogers 2003). There, diffusion is defined as a phenomenon that occurs depending on the characteristics of the adopter. Further advancements and established theories integrate additional aspects that influence the adoption rate specified per application. Aspects such as social structures and mutual influences (Valente 1996), as well as acceptance issues and monetary factors, affect adoption patterns, often following an S-curve (Geroski 2000; Faber et al. 2010). The adoption over time that leads to the S-curve scheme is often split into five phases that have already been extensively discussed and reviewed in the literature (Barreto & Kemp 2008; Rao & Kishore 2010).

Kiesling et al. 2012 reviewed approaches for innovation diffusion and mainly distinguished between aggregate models and individual level models. Following this definition, aggregate models are more related to early modelling approaches in forecasting the diffusion of single product innovations in homogeneous social systems. In general, those statistical theory-based diffusion algorithms reflect the innovation diffusion in Rogers' theory (Rogers 2003). Numerous aggregated diffusion models exist, and several reviews have already studied the different approaches for various applications, e.g. Rao & Kishore 2010 for renewable energy technologies. The Bass model is still one of the best known, as it enables simple implementation based on a clear mathematical structure with few parameters (Bass 1969). However, extended versions can become complex, but especially heterogeneity of the adopters is difficult to represent in such an aggregated approach.

In contrast, individual level models allow for a better representation of heterogeneity but require more extensive parameterisation and data. Heterogeneity is considered through the granularity of individual decisions that are influenced by simple rules on behaviour and interactions. Meanwhile, it is also proposed to increase sensitivity by implementing dynamic parameters and considering multiple potentially competing innovations simultaneously. Regional aspects are often neglected by aggregate models, but have been proven to have a substantial impact on adoption patterns covered by individual level models (Barreto & Kemp 2008). Thus, since spatial attributes have an impact on diffusion behaviour, it is reasonable to build on individual level models, which allow a better representation of spatial aspects.

2.4 Diffusion methods in energy system modelling

Modelling the diffusion of the various components within an energy system is still a complex task. The dependencies between the energy supply, energy infrastructure, and energy demand sectors influence decision making. The methodological approach in energy system studies to connect sectoral dependencies within the given targets is often similar:

1. Investigating transition to achieve the sectoral goals of the demand sectors.
2. Integrating sectoral data on projections of energy demand in energy system models.
3. Connecting and balancing energy supply and demand using infrastructure models.

Energy system studies are often conducted for a specific time horizon and goal, such as reaching climate neutrality in Europe until 2050. Starting with demand models, they usually rely on a set of input data. These input data are available mainly only on the national level, including legislative regulations. Legislative regulations often form the framework conditions for the sectors involved. Examples are:

- Fit-for-55-package: Emission reduction targets of 55% until 2030 compared to 1990 (European Commission 2021).
- RFNBO quota: 42% of the industrial hydrogen demand from RFNBO until 2030 (European Commission 2022b; Motola et al. 2023).
- RED III: 29% RES in the transport sector or 14.5% emission reduction (European Commission 2023b).
- ReFuelEU Aviation: A total share of 6% sustainable aviation fuels (SAF) until 2030 and 70% until 2050 (European Commission 2023a).
- RePowerEU: 45% RES in the residential sector until 2030 (European Commission 2022a).

Most energy systems studies assume these quotas to hold, leading to predefined milestones in the development of respective pathways in scenarios.
The scarce availability of detailed data and the restrictions from the regulatory framework typically result in exogenous definitions of the main drivers for the diffusion of new technologies or processes at the national level. Demand models deliver national demand projections based on exogenous assumptions to energy system optimisation models, which primarily cost-optimise power plant capacity to meet the calculated demands. However, optimisation of those power plant capacities is often also limited by constraints, such as regulatory development goals for the expansion of renewable energy.
Thus, the diffusion on the energy supply side is mainly impelled by the previously calculated demand data and exogenous development targets on the expansion of renewable energies and national legislation. The calculations for the expansion of energy infrastructures, such as electricity grids and gas networks, are then carried out subsequent to the regionalisation of national demand and supply quantities. In conclusion, the results from demand modelling actuate the general diffusion across the model chains but are currently often assumed exogenously on national level based on legislation. In addition, for industry, huge investments, long investment cycles, as well as the availability of energy carriers and infrastructure should also be considered to investigate process diffusion (Wesseling et al. 2017).

2.5 Diffusion methods in energy demand modelling

Implemented as part of IAMs or ESMs in energy system studies, demand sectors are often not the focus of detailed investigations. Thus, the representation of the demand sectors within those frameworks is relatively simple, and generic trends based on assumptions are fed exogenously. The diffusion algorithms typically follow equations and distributions that describe the adoption phases following a typical S-curve (Geroski 2000). Predetermined regulations translate to exogenous assumptions and reference points, which form the exact course of the diffusion curves. Thus, these models are reflected in the aggregated approaches described by Kiesling et al. 2012. To overcome some weaknesses of these aggregated sectoral representations, some documentations on integrated demand sector approaches within IAMs and ESMs describe the implementation as an agent-based approach. Sectoral demand agents interact through economic interactions with other agents and modelled energy markets. However, these approaches do not depict individual decision makers, but rather describe representative entities of a sectoral group per region. The representative entity embodies a group of individuals with statistical shares of various characteristics. However, because of the statistical aggregation of characteristics and the loss of individual resolution, this type of representative modelling still belongs to the aggregate models. Representation as an aggregate model at the national level using representative entities is a valid, logical, and sensible approach due to the availability of data mentioned in section 2.4. The disadvantages of incorporating representative agents, which is a widely used approach within ESMs, are further analysed by Rubiano Rivadeneira & Carton 2022. This representative approach is often referred to as agent-based modelling in the literature and is used not only within IAMs and ESMs but also for dedicated demand models of a single sector. Examples include the number and type of vehicle per household in the transport sector (Zhang et al. 2011; Higgins et al. 2012; Gnann & Plötz 2015; Mehdizadeh et al. 2022), the spread of energy efficiency measures in residential buildings (Moglia et al. 2017; Sachs et al. 2019; Papadopoulos & Azar 2016; Niamir et al. 2020), or the type of plant to manufacture a specific product in the industrial sector (Moya et al. 2020; Budinis et al. 2020). More detailed information and thorough reviews of well-known demand modelling approaches (Suganthi & Samuel 2012; Pfenninger et al. 2014) and comparisons of IAMs and their transparency and comparability are available in further literature (Capros et al. 2014; Nikas et al. 2021b; Nikas et al. 2021a; Giarola et al. 2021). Although Rubiano Rivadeneira & Carton 2022 highlight the disadvantages through the assumed average equality of individuals within the groups, this approach also offers many advantages. A large group with similar properties can be described with limited data and covers a wide range of essential influencing factors. In addition, the aggregation makes it computable sufficiently within complex optimisation problems of IAMs and ESMs.

However, due to the aggregations, spatial accuracy, and individual criteria within these groups are lost. Moreover, it is not possible to draw conclusions on the combination of temporal and spatial development since the individual members of the representative group cannot be delineated.

2.6 Diffusion methods in industry sector models

As previously introduced for diffusion patterns in energy system modelling, public statistics and databases also serve the basis for assessing the industry sector. The industry sector is enormously heterogeneous with many different actors due to a broad range of branches, products, and processes. However, the modelling detail in most IAM and ESM implementations is constrained to the branch level due to the limited availability of more granular public data. Contrary to those sectoral aggregation methods of IAMs and ESMs, some studies conduct bottom-up analyses on the industry sector. While some focus only on technical or techno-economic investigations of single processes (Vogl et al. 2018; Ikäheimo et al. 2018), others assess model-based scenarios on different branches like iron and steel (Richardson-Barlow et al. 2022; Harpprecht et al. 2022; Schneider 2022), or products, e.g. glass (Zier et al. 2023 or cement (Schneider et al. 2023).

The most detailed existing bottom-up industry models applied at the European level are FORECAST (Fleiter et al. 2018), IndustryPLAN (Mathiesen et al. 2023; Johannsen et al.

2023), and WISEE-EDM-I (Schneider et al. 2020; Kloo et al. 2024).
WISEE-EDM-I is very detailed for specific sectors, but does not cover the entire industry. However, it enables an optimisation of production networks and industry clusters for steel and chemicals. The calculated production networks from WISEE EDM-I show site-specific resolution.
IndustryPLAN covers all industry branches, but is not detailed on the industrial production networks and spatial resolution. The products with the highest share of energy demand are explicitly considered, while further applications are calculated with an aggregated and general approach. The calculated results on energy demand and other indicators reflect national resolution.
FORECAST calibrates to national energy balances. It has a unique method for breaking down the energy demand for the entire industry into individual processes. Subsequently, FORECAST provides a regionalisation approach to distribute the national demand data to NUTS3 regions. This provides a better technological and spatial resolution than IndustryPLAN or other tools with national resolution for the entire industry, but a more aggregated view on individual products than WISEE EDM-I.
The models, as well as industry sector representations within IAMs and ESMs, have in common that sector-specific activity data, such as industrial production, define exogenous diffusion pathways. Based on defined pathways, the models allow for a bottom-up simulation of industry transition according to the exogenous inputs.

Following, the FORECAST-Industry model is briefly presented with more detail as it was used for some co-author work within this thesis. Within FORECAST, i.e. fuel switch for industrial process heat (Rehfeldt et al. 2018; Rehfeldt et al. 2019; Rehfeldt et al. 2020), is based on a discrete choice simulation (Fleiter et al. 2018). The aggregated national plant capacities are initialised using a stock approach that allocates a statistical age distribution (Weibull distribution). Thus, the average plant ages and national dissemination curves can be estimated without knowledge about individual industry sites. The minimum and maximum market shares of each possible process per product and year at the national level are defined exogenously. Within these predefined shares, the model chooses between alternative processes. The stock approach represents the heterogeneity of industry and ensures that no complete market share is achieved by one technology (Fougeyrollas et al. 2019). Assumptions on key drivers for economic competitiveness, such as energy carrier price paths, define different scenarios to draw conclusions about future developments. The parameterisation of conventional and alternative processes is based on values from scientific literature. Across the different industry branches, numerous investigations and analysis exist both at systemic and highly technological level. Detailed technical studies deliver process parameterisation, while systemic studies often contribute economic data. The data used in the existing models, as well as the work conducted within this thesis, is highly dependent on those previous studies. Some of the most important scientific publications across the various branches and processes in recent years are listed and summarised in Table 1.

In summary, the current state of industry models focuses on the competitiveness of conventional and alternative processes. The aim and value of industry sector models is to highlight the key challenges of industry transition to conclude on robust future developments. The most important aspects to be quantified for addressing future uncertainties and to guide energy planning are:

- Energy demand projections
- Process diffusion behaviour
- Economics and transition costs
- Policy effectiveness
- Spatial resolution
- Infrastructure connection

Energy demand projections: One of the biggest uncertainties in industry transition is the future development of energy demand per branch and respective energy carrier (Fleiter et al. 2018). Investigations on energy demand projections depending on different future developments by conducting scenario analysis are crucial for energy planning strategies (Pfenninger et al. 2014; Reveron Baecker et al. 2025). Historical energy balances are provided by public organisations, such as Eurostat (Eurostat 2025) for the European countries or individual national organisations, i.e. AG-Energiebilanzen (AGEB 2024) for Germany. Industrial energy demand and type of energy carriers is highly dependent on the annual production output and used processes for manufacturing. The type of process determines the techno-economic parameters, such as the specific energy consumption (SEC), capital investments, operational costs, and the necessity for various energy carriers.

Process diffusion behaviour: The process diffusion behaviour is the influencing factor of the resulting energy demand projections. The diffusion of new innovative and climate-neutral processes into the industrial plant stock depends on a variety of parameters (Fleiter et al. 2018). First, the technology readiness level (TRL) of a process determines its commercial availability or the starting point of possible future market adoptions. Additional factors influencing process diffusion include specific individual considerations, such as the age of the current plant stock and the lifetime of the processes, as well as the availability of energy infrastructure (Wesseling et al. 2017). Economic competitiveness, influenced by the techno-economic parameters of the process and the associated costs of the required energy carriers, drives the transition between processes (Groppi et al. 2025).

Economics and transition costs: Apart from the above mentioned restrictions (TRL, infrastructure connection) economic indicators are the key decision criteria. Process-specific data on capital expenditures (CAPEX), operational expenditures (OPEX), as well as material, feedstock, and energy demand impact on the economic competitiveness (Hörbe Emanuelsson et al. 2025). The highest cost shares are, in most cases, related to material and energy provision. Current and future energy prices determine the economic competitiveness and transition costs among the different processes available (Samadi et al. 2023). Therefore, assumptions on the future developments and projections are sensitive parameters in energy system models. In addition, the political framework and penalties, such as CO_2-prices, further affect the costs of production (Hörbe Emanuelsson et al. 2025).

Policy effectiveness: Energy transition policies significantly impact energy planning and economic competitiveness. Currently, some policies still support the use of fossil energy carriers, and statistics even show an increase in subsidies spent in most European countries in 2023 compared to 2015 (European Environment Agency 2025). However, to force the energy transition, these old policies are abolished and, instead, new policies are established that support renewable energy and climate neutrality (Sreekanth 2024). These policies, which are designed to shift from fossil fuels to renewable sources, necessitate rethinking energy generation, distribution, and consumption. The effectiveness of the new policy incentives is tested and evaluated through implementation in model-based scenario analyses (Süsser et al. 2021). Successful policy frameworks balance cost penalties between conventional and alternative processes with long-term benefits such as reduced greenhouse gas emissions and increased security of energy supply.

The four above mentioned aspects are already covered, at different aggregation levels, by existing modelling approaches. However, due to the lack of sufficient spatial resolution, infrastructure connection is mostly neglected or cannot be assessed by current models.

Spatial resolution: Current energy system models often operate at national level or based on node aggregations, which is often limited by accessible public data, legislative regulations, and computation capacities, as described in section 2.6 (Fattahi et al. 2020; Martínez-Gordón et al. 2021; Fodstad et al. 2022). However, the importance of spatial resolution of the scenario results is substantial and is gaining progressively more attention in the community and decision making (Martínez-Gordón et al. 2021). Especially innovative industry processes need access to climate-neutral energy carriers, e.g. hydrogen, and rely on a secured energy supply. Thus, the diffusion of innovative processes depends on a variety of site-specific and regional preconditions. Examples that highlight the need for high spatial resolution in industry models include infrastructure access, energy carrier prices, the age of existing plants at an individual industry site, and political frameworks.

Infrastructure connection: Infrastructures and logistics, such as pipelines, electricity grids, railways, or truck supply, are established and sufficient for fossil energy carriers and conventional fossil-based processes. However, the energy transition, and industry transformation in particular, requires huge amounts of climate-neutral energy carriers (Fleiter et al. 2024a). Thus, industry sites need access to the corresponding energy infrastructure, which is a prerequisite to make investment decisions for climate-neutral processes. In addition to the direct use of renewable electricity and the resulting need to expand electricity grids, hydrogen and its derivatives are seen as the most promising energy forms (Neumann et al. 2023; Wietschel et al. 2024). However, today there are hardly infrastructure and logistics for hydrogen transport (Hydrogen Tools 2016). Regardless of the challenges on the supply or demand side, infrastructures play a crucial role in strategic energy planning to link the respective sectors. Initiatives like the European Hydrogen Backbone (EHB) present first plans to ramp up hydrogen infrastructure in Europe (European Hydrogen Backbone 2021; European Hydrogen Backbone 2022).

Table 1: *Relevant scientific literature that provides quantitative and qualitative analyses focussing on single products of the energy-intensive industry branches.*

Product(s)	**Reference**	**Summary**
Ammonia	Ikäheimo et al. 2018	Analysis of Power-to-Ammonia plant and techno-economic description of the process
Ammonia	Nayak-Luke et al. 2018	Model-based calculations for green ammonia production costs and sensitivity analysis to determine the significance of different variables and plant size in production costs.
Ammonia	Armijo & Philibert 2020	Case study for green ammonia production based on renewable electricity in Chile and Argentina with transparent assumptions on the techno-economic process characterisation.
Ammonia	Zhang et al. 2020	Comparison and techno-economic characterisation of green ammonia production processes and their cost components and production costs.
Ammonia	Chehade & Dincer 2021	Comprehensive, relatively low-threshold overview over all possible future ammonia value chains on production and demand side based on scientific literature.
Ammonia	Fasihi et al. 2021	Analysis of global ammonia production potentials of on-site and coastal production scenarios including techno-economic process characterisation, production costs, and shipping costs for green ammonia
Ammonia	Yüzbaşıoğlu et al. 2021	Low-threshold description and comparison of the various ammonia production methods that may be applicable at industrial scale in future.
Ammonia	Jain et al. 2022	Scenarios for cost analysis of electricity-based ammonia production and analysis of their revenues compared to market prices, as well as its sector coupling for use in food, energy, and trade sectors.
Ammonia	Del Arnaiz Pozo & Cloete 2022	Comparison and techno-economic evaluation for blue and green ammonia production based on three different production routes based on natural gas and one renewable process and sensitivity investigation for the critical variables for different countries.
Ammonia	Lee et al. 2022	Techno-economic evaluation of grey, blue, green, and nuclear-based ammonia production including process descriptions, cost analysis, GHG emissions and CO_2 avoidance costs.
Ammonia	Ausfelder et al. 2022	Grey literature on techno-economic description and scenario development on alternative hydrogen feedstock for ammonia production in Europe until 2030.
Ammonia	Ojelade et al. 2023	Review of the existing literature and summary of derived production costs of various green ammonia production processes.
Ammonia	Egerer et al. 2023	Comparison and techno-economic parametrisation of domestic grey and blue ammonia value chains and green imports from Australia.
Methanol	Jadhav et al. 2014	Description of methanol production from CO_2 and H_2, review of various catalysts as well as CO_2 conversion rates and improved methanol yield.
Methanol	Pérez-Fortes et al. 2016	Detailed investigation of CO_2 to methanol synthesis and techno-economic process description, cost analysis, and mass and energy balances.

Product(s)	Reference	Summary
Methanol	Zhang & Desideri 2020	Techno-economic performance and sensitivity analysis of equipment costs, full load hours, and energy and $CO_2$2 prices on alternative methanol production.
Methanol	Nyári et al. 2020	Model-based techno-economic investigation on green methanol production including mass balances analysing the impact of methanol price and H_2 on the NPV.
Methanol	Narine et al. 2021	Process flow diagrams of two fossil reforming (ATR & SMR) based and two alternative CO_2 based (pyrolysis & electrolysis) processes, techno-economic assessments, sensitivity analyses and life cycle assessments.
Methanol	Lonis et al. 2021	Technical assessment of two concepts for renewable methanol production into energy systems with improved thermal energy storage and heat integration.
Methanol	Kang et al. 2021	Summary and overview of several methanol production pathways with technical and economic parameterisation based on existing literature and lists of globally existing methanol plants and projects.
Methanol	Del Arnaiz Pozo et al. 2022	Investigation on four different methanol production routes based on natural gas or renewables and techno-economic process descriptions to assess sensitivity analysis for the critical variables for different countries.
Methanol	Kim et al. 2022	Analysis of four cases for methanol production based on natural gas, coal, renewables, and direct CO_2 electrolysis on carbon footprints and detailed costs depending on different plant scales.
HVC	Ren et al. 2006	Detailed investigations on conventional HVC production routes, their catalysts, energy and feedstock consumptions, emission balances, and product yields.
HVC	Ren et al. 2008	Review, detailed description, and comparison of conventional steam cracking and alternative MtO production route with respect to their energy demand, CO_2 emissions, and production cost estimations.
HVC	Dechema 2017	Grey literature containing extensive description of fossil, bio-based, hydrogen-based and other alternative processes and their techno-economic characteristics for the basic chemical industry, including ammonia, methanol, and HVC.
HVC	Spallina et al. 2017	Mass and energy balance for different olefin production routes complemented by an economic comparison of selected European plants.
HVC	Platt & Styring 2022	Review of different olefin production routes and indications of technical parameters, such as catalysts, reaction temperatures, and specific energy and feedstock consumption.
HVC	Zhang et al. 2023	Comparison of techno-economic indicators and environmental impacts, selling prices, and sensitivity analysis of two different Fischer-Tropsch production routes and the MtO process.
HVC	Abbas-Abadi et al. 2023	Review and description of fossil and renewable production pathways for light olefins and analysing chemical recycling through pyrolysis of plastics waste and catalyst performances.
HVC	Lopez et al. 2024	Techno-economic description of various HVC production routes including MtO and import value chains for different European countries with calculated production costs and life cycle assessment.
Primary steel	Vogl et al. 2018	Model-based techno-economic analysis of a H2-DRI process design that gives key parameters on different cost components, energy demand and emission intensity.

Product(s)	Reference	Summary
Primary steel	Vogl et al. 2020	Policy instrument evaluation and quantification with respect to their effectiveness, feasibility, and fairness for a transition of European steel making towards green steel production and conventional non-EU producers.
Primary steel	Vogl et al. 2021	Investigations on phasing-out global blast furnace plants and corresponding emission reduction potential based on the analysis of the average plant lifetimes per continent from historical and statistical data.
Primary steel	Müller et al. 2021	Modelling of a process design for H2-DRI using hydrogen from HT electrolysis and validation of technical parameters, such as SEC, with real operational data.
Primary steel	Zhang et al. 2021	Review and process descriptions considering real projects and field technologies in Europe, the USA, and Asia countries
Primary steel	Richardson-Barlow et al. 2022	Analysis of policies and pricing on the economics of different steel production process options for low carbon steel, including CCS options on blast furnaces and direct reduction using natural gas (NG-DRI), as well as H2-DRI with different scrap input and electric arc furnace (EAF) for secondary steel production,
Primary steel	Harpprecht et al. 2022	Investigation of four different primary steel and one secondary steel production routes in four different scenarios for Germany with narratives on a reference, electrification, coal-exit, and CCS within an applied carbon budget and analysed concerning their technology mix, energy demands, and implications on future energy supply.
Primary steel	Schneider 2022	Site-specific analysis of the plant stock in integrated primary steel production for sites in Northwestern Europe with a decision-based modelling approach for investments towards climate-neutral processes.
Primary steel	Shahabuddin et al. 2023	Review and techno-economic comparison of various process options for primary steel production and the integration of alternative H2-DRI and other low-carbon options.
Primary steel	Maier et al. 2024	Assessment of process options for primary steel production and the market diffusion in different world regions with an underlying analysis of individual companies and their strategies, perspectives and actions towards low-carbon steel production.
Cement	Schneider et al. 2011	Discussion of the different cement classifications, alternative raw materials, as well as energy demand of the individual production steps and their potentials for efficiency improvements, alternative fuels, and emission reduction and mitigation.
Cement	Aranda Usón et al. 2013	Investigation on the entire cement value chain from quarrying to transport of the end product and analysis of the use of waste and other alternative fuels and raw materials.
Cement	Rootzén & Johnsson 2017	Analysis of carbon cost impacts on cement production costs and the effect on the share of construction costs depending on the CO_2 allowance price.
Cement	Kermeli et al. 2019	Recommendations for better industry representation within IAM and application for the cement industry by implementing energy efficiency measures, retrofit options for improved process differentiation, and changes in the clinker to cement ratios.

Product(s)	Reference	Summary
Cement	Schneider et al. 2023	Description of a net-zero pathway for the cement production by applying and combining several mitigation levers, description of alternative fuel options, and comparison of carbon capture technologies and their impacts on production costs.
Cement	Müller et al. 2024	Implementation of efficiency measures and innovative clinker kiln systems, as well as alternative fuel mixes and improved clinker-to-cement ratios into IAM scenario pathways to assess their impacts on climate change and provision of techno-economic assumptions.
Cement	Williams et al. 2024	Assessment on the role of different configurations of hydrogen and oxyfuel combustion technologies in cement production on emissions mitigation and energy consumption.
Lime	Greco-Coppi et al. 2021	Process modelling of the integration of a carbonate looping CCS unit into a lime production plant and conducted sensitivities for different temperature to analyse emission reduction and energy consumption behaviours.
Lime	Simoni et al. 2022	Description of state-of-the-art lime production processes and possible process options, especially for emission mitigation using CCS, but also fuel switch to avoid energy-related emissions.
Lime	Laveglia et al. 2023	Carbon direct avoidance (CDA) through energy efficiency measures and alternative fuels, as well as CCS options in lime manufacturing as part of a life cycle assessment on the impact of cradle-to-gate emission in construction materials.
Lime	Greco-Coppi et al. 2024	Process modelling of different CCS concepts (retrofit versus integration), fueling types, and heat integration to assess the impact on CO_2 avoidance costs.
Glass	Zier et al. 2021	Detailed description of different glass types and manufacturing processes and specification on technical parameters, such as SEC, as well as review of different process and fuel options to decarbonise.
Glass	Griffin et al. 2021	Assessment of glass decarbonisation options in a hybrid top-down and bottom-up modelling approach of the UK industry landscape considering a policy-oriented and systemic perspective.
Glass	Del Furszyfer Rio et al. 2022a	Extensive review of the glass manufacturing process step and their respective technology options based on the existing literature and projects, as well as the implications and barriers of costs and social behaviour.
Glass	Caudle et al. 2023	Investigation on the integration of CCS technologies in different cases and the results of the simulation model on the achieved emission mitigation and costs.
Glass	Barón et al. 2023	Presentation of low-carbon glass making concepts and detailed analysis of calcium-looping capture systems in combination with the use of synthetic methane from green hydrogen as alternative fuel option.
Glass	Zier et al. 2023	Bottom-up modelling and analysis of different scenarios for glass decarbonisation pathways for Germany with a focus on fuel switch to hydrogen or electricity-based process options.
Paper	Laurijssen et al. 2012	Investigation on energy costs and emission intensities for various energy conversion and supply technologies based on different energy carriers applied to three European countries (NL, SE, PL).

Product(s)	Reference	Summary
Paper	Fleiter et al. 2012	Model-based analysis of energy efficiency measures in the German pulp and paper industry with a focus on SEC, technology diffusion per process step, emission mitigation potentials, and corresponding difference costs for production.
Paper	Scordato et al. 2018	A Swedish case study that focuses on policy options and a suitable policy mix to support a sustainable transition in the pulp and paper industry.
Paper	Griffin et al. 2018	Fuel switch towards bioenergy, energy efficiency improvement and heat recovery as well as demand side flexibility to assess a technology roadmap for the UK pulp and paper industry.
Paper	Lipiäinen et al. 2022	Analysis of historic values from 2002 until 2017 concerning energy consumption, energy efficiency, and CO_2 emission reduction as well as conclusions and projections of future tendencies from the historical trends.
Paper	Del Furszyfer Rio et al. 2022b	Extensive review of the pulp and paper industry with a short analysis on energy use and climate impact for many European countries and discussion on decarbonisation options per process step, such as energy efficiency measures, electrification and CCS options, and improved circular economy.
Paper	Mati et al. 2023	Research of on-site electrolysis combined with the use and implementation of hydrogen in CHP plants to decarbonise the pulp and paper industry and description of the techno-economic assumptions.
Refineries	Vogt & Weckhuysen 2024	A thorough assessment of future sustainable refinery configurations using waste, biomass, CO_2, and hydrogen as feedstocks based on mass balances for an estimated scale-up.

2.7 Motivation for site-specific industry modelling

This thesis is motivated by enhancing the representation of the industry sector in energy system modelling tools to improve spatial resolution and diffusion dynamics. Therefore, methodological novelty by implementing an individual-level site-specific approach captures spatial and timely dynamics. The developed approach aims to address some of the barriers to industry transition identified by Wesseling et al. 2017 and already listed in section 1, such as the limitation by plant age and lifetime. The results provide a new level of detail through consideration of individual industry sites and their characteristics on plant capacity and plant age. A sustainable industry transition and highly spatially resolved data enable more reliable strategic energy and infrastructure planning.

Second, sufficient implementation of a hydrogen economy in the energy system requires integrated planning of all involved stakeholders. For an economic and sustainable European energy transition, especially in the industry transition, hydrogen will certainly play an important role with significant shares in future energy demand. Although direct electrification is expected to be the more efficient and economical decarbonisation option for a broad variety of industry applications (Sorknæs et al. 2022), technical maturity for some processes is still low (Fleiter et al. 2024b). Especially H2-DRI for primary steel production and climate-neutral feedstocks for the chemical industry will rely on the supply of green hydrogen. In addition, indirect electrification by using green hydrogen from electrolysis may offer some advantages and can help overcome some barriers of direct electrification that exist particularly for HT processes. While some of the co-author publications also assess possible future pathways through direct electrification in the industry sector, the focus of this thesis is to investigate hydrogen-based processes.

In summary, three key statements can be derived:

1. Detailed considerations of hydrogen-based processes as alternatives to conventional fossil-based production across energy-intensive industry branches are missing at the level of energy system analysis.
2. Existing modelling approaches for the industry sector do not show a sufficient spatial resolution. Industries account for huge amounts of energy demand and the transition towards climate neutrality will result in substantial changes. Future demand for renewable energy carriers, such as hydrogen, may occur at hotspots at a few sites and is therefore unevenly distributed. This poses challenges for the supply side and the corresponding infrastructures. Especially the interplay between energy supply and demand by considering infrastructures and their representation in energy system modelling necessitates detailed research.
3. The diffusion of new processes highly depends on their techno-economic properties, but also on the age structure of the current plant stock, which can be translated into the need for reinvestments. The timing of the investment decision is determined by the age and reinvestment cycles of the production units (Wesseling et al. 2017). The combination of evaluating process costs and reinvestment cycles together with infrastructure availability is crucial because the market in most industrial sectors is determined by long lifetimes posing the risk of fossil lock-ins. Thus, the age structure of the current plant stock allows reliable assessments on the speed of possible transformation pathways and the diffusion of hydrogen-based processes.

3 Problem statement

Several models exist to analyse the impacts of different factors on the energy system and future developments, such as policies and energy prices. Section 2 gives an overview of the various approaches, aggregation levels, and model types. The assessment of climate neutrality in industry is one part of these modelling activities, as heavy industries like steel and basic chemicals face challenges in transitioning towards a climate-neutral production. Diffusion theories try to understand and predict the adoption and future market dynamics of innovations. However, the implementations of diffusion patterns in existing models face challenges in capturing realistic spatial and temporal diffusion dynamics due to missing data and methods. Some so-called agent-based implementations exist for the demand sectors, but all implementations are based on representative entities as aggregated models that lead to loss of individual and spatial characteristics.

3.1 Drivers for investment decisions and site-specific spatial resolution

For process diffusion in industry, especially monetary factors, energy savings, and emission mitigation play a role. However, due to political climate targets and corresponding constraints from legislative regulations, the diffusion of climate-neutral processes in existing approaches is defined exogenously. This may reduce to some extent the complexity of decision-influencing factors, but, on the other hand, makes established diffusion theories unfeasible for predicting process diffusion. Industrial processes require huge capital investments, so the economic process switch depends on plant age and lifetime of industrial processes (Wesseling et al. 2017). However, in current approaches to model the industry sector, exogenous assumptions such as linear shutdown profiles or other statistical distributions are used to estimate diffusion pathways. These aspects indicate the need for a new methodological approach to address the hurdles in the diffusion of industrial processes and the corresponding research questions. To define proper research gaps for further analyses of industrial transformation, Wesseling et al. 2017 investigated barriers to innovation in energy-intensive industries. In summary, long investment cycles lead to few windows of opportunity to invest in climate-neutral processes and reduce investment capital through low cyclical profit margins. In addition, incremental improvements of the core process technologies and the risk of losing market shares due to failure in investment decisions support lock-ins. The main bottlenecks are stated to be costs and availability of energy carriers and infrastructure. For these reasons, the priority of the main drivers of technology diffusion in industry is shifted to the age of production units and reinvestment cycles compared to conventional diffusion theories. The choice among competing alternative process options is basically driven by techno-economic factors in cooperation with spatial preconditions. Current models used to evaluate industry transition pathways commonly have limited spatial detail. Combining individual investment decisions with a site-specific spatial resolution contributes to closing the research gap on the spatial and temporal dynamics of industry transition scenarios. In summary, there is a need for spatially highly resolved results to inform decision makers about strategic energy planning, for example, establishing new hydrogen and CO_2 infrastructures.

3.2 Objectives and research questions

The key objective of this thesis is to address several challenges in modelling hydrogen-based processes in energy-intensive industries, as highlighted in the previous chapters.

Key objective: ***Improve the spatial and timely resolution in industry demand modelling on the example of hydrogen-based processes for energy-intensive industries.***

The lack of comprehensive technical data complicates the accurate representation of hydrogen-based processes in transition pathways. Therefore, *RQ* 1 aims to bridge the gap in key technical parameters necessary for accurately modelling hydrogen-based processes.

***RQ* 1**: **What is the technical potential of hydrogen-based processes in energy-intensive industries?**

***RQ* 1.1**: *Which hydrogen-based processes may be applicable in the energy-intensive industry branches?*

***RQ* 1.2**: *What are the technical characteristics of the hydrogen-based process alternatives to assess the technical hydrogen potential?*

A high spatial resolution in industry modelling helps to capture the precise distribution of energy demand. This allows for more accurate planning of energy infrastructures, such as hydrogen pipelines. The highly resolved spatial results derived from *RQ* 2 can help identify bottlenecks and allocate regional differences in availability and demand to find appropriate solutions from an energy system perspective.

***RQ* 2**: **How could the spatial and timely transition towards hydrogen-based processes be captured in energy demand modelling?**

***RQ* 2.1**: *How do individual site-specific investment decisions of primary steel and basic chemical sites affect the spatial distribution of hydrogen demand?*

***RQ* 2.2**: *Are current plans for hydrogen infrastructure sufficient to meet hydrogen demand of primary steel and basic chemical sites?*

The age and structure of the current plant stock have a significant impact on the economic viability of market diffusion. However, alternative processes are often more expensive than existing fossil-based production, making market acceptance difficult. Techno-economic and spatial factors determine the diffusion dynamics, targeted by *RQ* 3.

***RQ* 3**: **What techno-economic factors determine the diffusion dynamics towards hydrogen-based processes for primary steel and basic chemical production?**

***RQ* 3.1**: *How do plant age, lifetimes, infrastructure access, and economic competitiveness to fossil production affect the timely and spatial diffusion of hydrogen-based processes?*

***RQ* 3.2**: *How do hydrogen and CO_2 prices influence competitiveness and site-specific investment decisions?*

4 Research approach

As introduced in section 1, hydrogen is a promising energy carrier for future applications, which can be used for both feedstock and energy purposes. The focus of this dissertation is on the energy-intensive industry branches, in particular hydrogen-based processes as alternatives to conventional production.
A review of the state of industry modelling within the research field of energy system analysis before this work is presented in section 2. In summary, previous studies investigating the industry sector did mostly not reflect on the following three important aspects, or at least did not reflect on them all together.

1. **Techno-economic characterisation** of hydrogen-based processes (*RQ* 1).
2. **Site-specific spatial resolution** and infrastructure dependencies (*RQ* 2).
3. **Plant age and reinvestment cycles** for process diffusion (*RQ* 3).

Having outlined the motivation for the methodological enhancements within this dissertation, the objective and related research question to improve the modelling of the spatial resolution and process diffusion dynamics of the industry sector are extracted in section 3. The key objective is broken down into smaller research questions, and this thesis rebuilds them back into the central theme. Therefore, Figure 3 shows the connection of the publications to the respective research questions and their type of contribution. The papers of my core publications are directly related to the key objective and research questions. Apart from the core publications (Papers 1, 2, & 3), the further main author (Papers I & II) and co-author publications (Papers A, B, C, D, & E) contribute to parts of the research questions and support this thesis with background knowledge. The individual papers are dedicated to the research questions as follows:

RQ 1: Paper I focuses on a first bottom-up assessment of integrating green hydrogen in the German chemical industry.
Subsequently, Paper 1 investigates hydrogen-based process options for the entire energy-intensive industry branches and assesses the techno-economic properties of hydrogen-based processes.

RQ 2: Paper II represents a first simple approach to consider site-specific reinvestment cycles for the diffusion of hydrogen-based production for northwest European countries. Following this approach, Paper 2 describes the method of the finally established site-specific model to conduct scenario analysis that delivers thorough results on indicators of industry transition pathways.
The co-author Papers A and B contributed to the data basis and methodological developments, while Papers C and E confirm the focus on the selected products.

RQ 3: Based on the established model from *RQ* 2 and Paper 2, Paper 3 analyses the diffusion of hydrogen-based primary steel and basic chemicals production in Europe. Depending on plant ages, infrastructure availability, and varying prices of hydrogen and for CO_2 certificates, site-specific investment decisions lead to different transition pathways. The co-author Papers C, D, and E and their analysed scenarios support the need for spatially accurate hydrogen demands and realistic diffusion dynamics for the focused products.

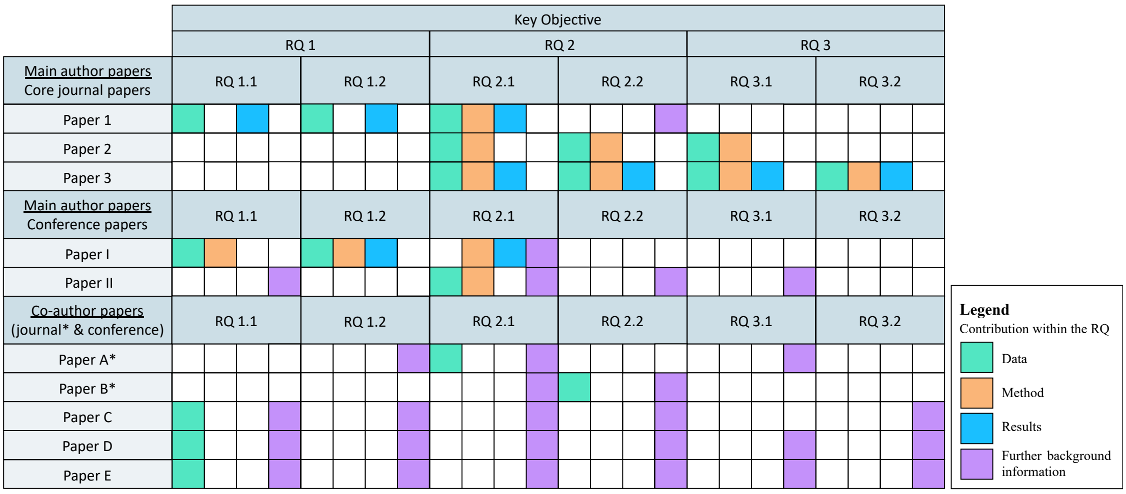


Figure 3: *Overview over the connection of the publications within this thesis and the raised research questions.*

4.1 Techno-economic characterisation of hydrogen-based processes

In the first step, *RQ* 1 requires a thorough understanding of the processes and their research status. Some investigations in energy system studies considering high hydrogen demands for industry transition pathways were conducted before the start of this thesis in 2020. However, the data on processes and the resulting analyses were on fairly aggregated levels and showed huge bandwidths that represent high uncertainties. Some applications, especially in the chemical industry, already use hydrogen as an intermediate converted from fossil energy carriers - mostly natural gas by steam methane reforming (SMR) (Fleiter 2013; Dechema 2017). For these basic chemicals, the provision by electrolysis from renewable electricity appears to be a technically relatively easy market entry for green hydrogen (Dechema 2017).

A first plant-specific bottom-up estimation is conducted in Paper I to decarbonise the German basic chemical industry based on simplified techno-economic assumptions. The feasibility of using hydrogen in other industry branches for process heat applications was much more uncertain. Therefore, continuing to *RQ* 1.1 and *RQ* 1.2, a thorough literature research was conducted to identify the relevant processes in energy-intensive industry branches and quantify their techno-economic properties. Many of the scientific publications covered are listed in Table 1 in section 2.6. The required process temperatures, the corresponding TRLs of the hydrogen-based process alternatives, and the respective estimates of the specific hydrogen consumption (SHC) were investigated in Paper 1.

4.2 Site-specific spatial resolution in industry transition

During the work of Paper 1 for the site-specific hydrogen demand potentials, the Fraunhofer ISI IndustrialSiteDatabase on European industry sites is co-established, extended, and validated. The maintenance and development of the Fraunhofer ISI IndustrialSiteDatabase is a permanent task during the course of this thesis. The application and matching of specific hydrogen demand estimates with the industry database led to a bottom-up estimation of the site-specific technical future hydrogen potential of energy-intensive industries in Germany (Paper 1). In combination with a top-down approach for the remaining industries, the technical maximum potential and the mitigation of GHG emissions were analysed. However, no diffusion pathway or a timely reference for the potential hydrogen demand is given. The published open data set was widely accepted by the community in this field of research and was taken several times to perform further analyses (Lieberwirth & Hobbie 2023).
A method was established within the sEEnergies project to estimate industrial excess heat at various temperature levels for all sites included in the Fraunhofer ISI IndustrialSiteDatabase in Europe. Details are presented in Paper A, and - in terms of progress for this thesis - a validation for all European sites included in the database took place. In subsequent work, additional parameters regarding plant age and process lifetimes were added to enhance the determination of diffusion pathways for hydrogen-based processes, according to *RQ* 2. A qualitative analysis in Paper B elaborates on the dependence of the energy-intensive industry branches on the gas transport network. Research on individual industry sites provides plant ages (*RQ* 2.1) and helps estimate remaining reinvestment opportunities (*RQ* 2.2), along with the resulting spatial distribution and infrastructure dependency. An initial modelling approach in Paper II indicates the first attempts to integrate hydrogen diffusion pathways in northwest European countries. Plant age and lifetime determine the diffusion, but this approach neglects economic factors, as well as comparisons and competitiveness with conventional fossil-based processes. However, the site-specific hydrogen potentials serve as a spatially highly detailed basis for further research on industry transition pathways. This approach was the basis for the development of a more complex and comprehensive site-specific industry model.
Primary steel production and basic chemicals are found to be the most robust industrial hydrogen demanders and show the highest TRL for their respective hydrogen-based process alternatives. This observation is strengthened by the results derived within the co-author contributions in the Papers C, D, and E. Therefore, these branches were chosen for more detailed investigations towards *RQ* 2.1 and *RQ* 2.2. In addition, those products show completeness on plant ages and production capacities in the Fraunhofer ISI IndustrialSiteDatabase. Other industries, such as glass or paper, have a much larger number of sites, making it difficult to obtain complete data on plant age and capacity for the entire branch. The annex in Paper 3 lists the European primary steel, ammonia, methanol, and HVC sites and the respective sources of manual research. To close the identified gaps in section 2 on the spatial and timely dynamics of industry transition modelling, the development of a new site-specific approach in Paper 2 pursues *RQ* 2. By applying the site-specific modelling approach within Paper 3, *RQ* 2.1 and *RQ* 2.2 are answered for primary steel, ammonia, methanol, and HVC sites in EU27+3.

4.3 Plant age and reinvestment cycles for process diffusion

The site-specific model evaluates the transition of energy-intensive industry sites. Detailed knowledge of production units and information on capacities, plant age, and emissions enable the simulation of individual investment decisions. Dependencies on hydrogen infrastructure within an adjustable proximity are considered. Paper 2 presents the detailed methodology and mathematical formulation of the resulting site-specific approach, which is at the same time the core method of this dissertation. A short summary of the model is given below in section 4.4. The most sensitive parameters for investment decisions in the model are regulations, such as prices for CO_2 certificates, as well as projections of energy prices, and the availability of hydrogen infrastructure. The timing of the investment decision is determined by the age and reinvestment cycles of the production units. The total cost of production serves as the main decision criterion to simulate individual investment decisions.

The model is published fully open source in line with Paper 2. Data collection on techno-economic process assumptions, derived from the sources in Table 1, and the established Fraunhofer ISI IndustrialSiteDatabase feed the model as input. Paper 3 addresses the research questions *RQ* 3.1 and *RQ* 3.2 by applying the model to evaluate and investigate transition pathways for primary steel, ammonia, methanol, and HVC. Projections of hydrogen-based process diffusion pathways and the corresponding key parameters are analysed, such as different cost components, the energy demand per energy carrier, and emissions. The calculation of difference costs and the resulting cost gaps between conventional fossil processes and hydrogen-based production indicates the resulting investment gaps between scenarios with low and high hydrogen prices. In addition, Paper 3 indicates the site-specific spatial development of energy demand per energy carrier based on theoretical reinvestment cycles for a sensitivity with low hydrogen and high CO_2 price projections. To answer the research questions *RQ* 3.1 and *RQ* 3.2 on the influence of parameters on possible transition pathways, sixteen sensitivities on variations for hydrogen and CO_2 prices (four variations each) were investigated for a fixed set of fossil energy price series.

4.4 Model overview

As motivated in the previous chapters of this thesis, insights into industry transition with high spatial resolution is needed to inform decision makers about strategic energy planning. Especially the interdependencies of temporal and spatial diffusion of new processes and the availability of respective energy infrastructure are of high interest. Paper 2 describes in detail the site-specific open source framework developed for modelling energy-intensive industries. Following the model and its specifications are briefly summarised.

Model specification

Figure 4 represents an overview of the model, its inputs, influences on the investment decision and gained results. Different databases feed the model on the input side. In the current state, plans for a topology development for hydrogen infrastructure according to the plans from the EHB initiative are read. The industry database contains the industry sites to be modelled and their production units with knowledge about plant age and production capacity. The techno-economic database includes the definition of products and the parameterisation of considered process options. The model settings define which products are modelled in each simulation run and allow variations in the scenario definitions. Examples are varying energy price projections and the implementation of policies, such as CO_2-pricing or bans for process options. The framework is published open source in line with Paper 2 on GitHub. Data for European primary steel and basic chemical sites are delivered within this open source version as they were published as open data in line with Paper 3. In summary, the methodological advancement focuses primarily on two aspects:

- Site-specific spatial resolution to assess spatial attributes of industry transition, such as the availability of hydrogen infrastructure and site-specific energy demands, covering *RQ* 2.
- Consideration of industrial plants, their current age structure, and typical reinvestment cycles determine the timely aspect for the diffusion of hydrogen-based processes. This relates to *RQ* 3.

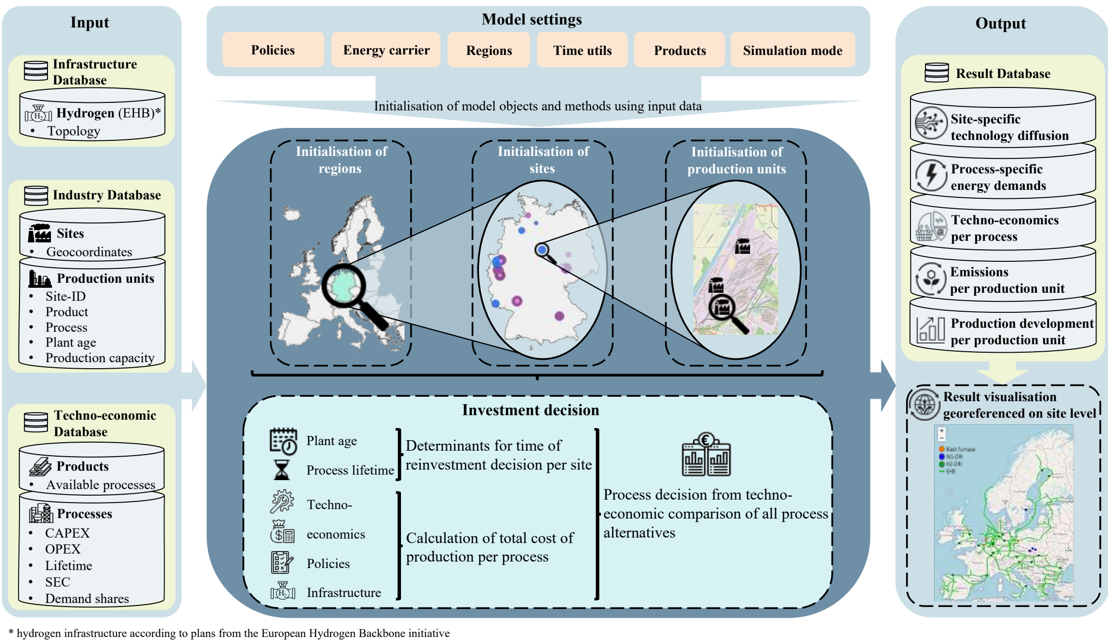


Figure 4: *Graphical abstract of the model methodology from Paper 2 (Source: Neuwirth et al. 2024b)*

The model stores the results of all variables in a result database. The outputs are given as time series for the energy demands and several cost calculations, such as investments, energy costs per energy carrier, emissions, and the corresponding costs for CO_2 certificates. These results allow for analyses of the diffusion of processes based on site-specific investment decision.

5 Key findings

This chapter highlights the key findings of the thesis. Figure 5 visualises the connection of the publications and represents the stepwise development towards the presented results.

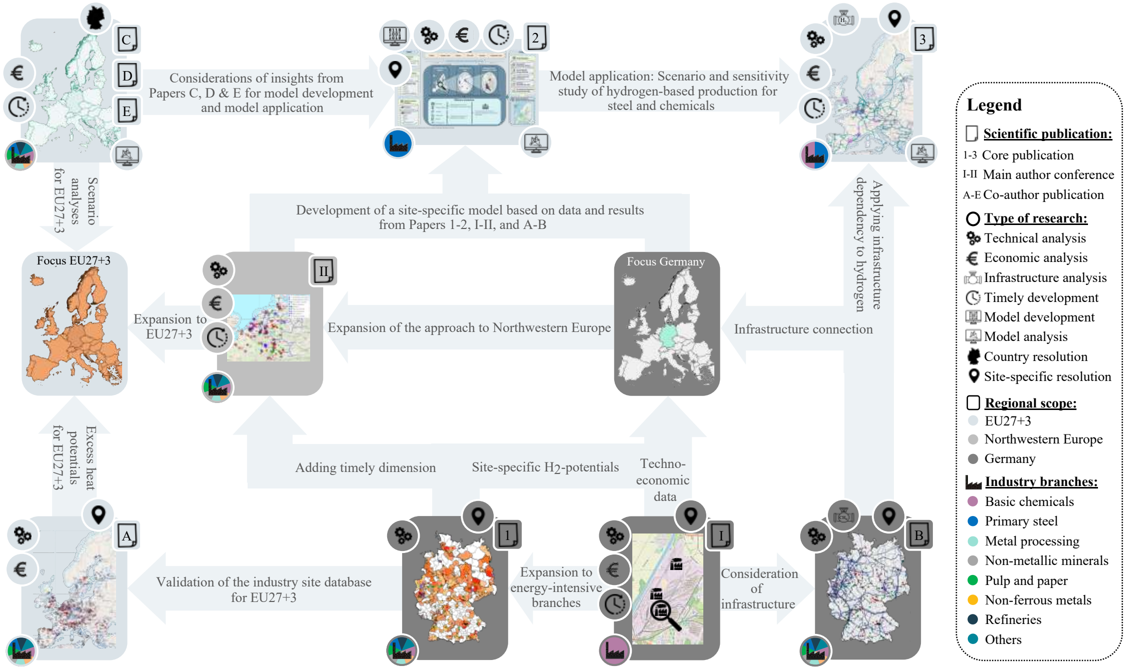


Figure 5: *Overview over the connection of the publications and the stepwise development of the method within this thesis.*

The four publications A, 1, I, & B at the bottom of Figure 5 (from left to right) describe the basis and the data collected. The analyses in the publications 1, I, & B have a strong focus on Germany, while the co-author publications on the left side (Papers A, C, D, E) focus on EU27+3. Paper II, which is an extension to Northwestern Europe based on the Papers 1 & I, represents an intermediate step in the methodological development. The data derived from the bottom papers and the insights from the co-author publications enabled the development of an open source industry model published in Paper 2. Finally, Paper 3 represents an application of the model and investigates sensitivities for hydrogen-based production of primary steel, ammonia, methanol, and HVC in the EU27+3.

5.1 Technical hydrogen potential in energy-intensive industries

What is the technical potential of hydrogen-based processes in energy-intensive industries?

Table 2 summarises the industry branches and products covered and indicates the TRL and specific hydrogen consumption (SHC) for hydrogen-based processes from Paper 1. From this overview, answering *RQ* 1.1, it is clear that hydrogen can be used for different

purposes in the energy-intensive branches. Some feedstock applications in the basic chemical industries for Germany were analysed in more detail in Paper I. High TRL is given for all feedstock applications and primary steel production. In those branches, alternatives are scarce. Low-temperature (LT) process heat, which is predominantly provided as steam, can also be provided using hydrogen at high TRL. However, direct electrification for these applications also shows technical maturity and is more energy efficient and economical (Sorknæs et al. 2022; Fleiter et al. 2024b). Hurdles still exist in specific HT applications due to different combustion properties compared to those of natural gas. In particular, the absence of radiant heat from hydrogen flames leads to uneven heat distribution and atmospherics. One of the most prominent examples is the difficulty in handling hydrogen in glass troughs leading to differing product properties (e.g., colour) compared to current manufacturing processes (Zier et al. 2021).
Additional techno-economic data derived from the literature in Table 1 pursue *RQ* 1.2.

Table 2: *List of covered industries within the Fraunhofer ISI IndustrialSiteDatabase and indication of TRL and SHC based on the lower heating value (SHC_{LHV}) in MWh per tonne of product from Paper 1 (Adapted from: Neuwirth et al. 2022a)*

Industry branch	**Product**	**Hydrogen use**	**TRL**	**SHC_{LHV}**
Basic chemicals	HVC	Feedstock	8-9	17.67
Basic chemicals	Ammonia	Feedstock	9	5.92
Basic chemicals	Methanol	Feedstock	8-9	6.31
Basic chemicals	Chlorine	LT process heat	8-9	0.86
Iron and steel	Primary crude steel	Reducing agent	8	1.89
Non-metallic minerals	Cement clinker	HT process heat	4-5	0.97
Non-metallic minerals	Flat glass	HT process heat	4-5	2.17
Non-metallic minerals	Container glass	HT process heat	4-5	1.28
Non-metallic minerals	Lime burning	HT process heat	3-5	1.03
Pulp & paper	Board & packaging paper	LT process heat	8-9	1.36
Pulp & paper	Tissue paper	LT process heat	9	1.92
Pulp & paper	Graphical paper	LT process heat	9	2.00
Pulp & paper	Recovered fibres	LT process heat	9	0.15
Pulp & paper	Chemical pulp	LT process heat	9	2.86
Non-ferrous metals	Aluminum, primary	HT process heat	4-5	1.90
Refineries	Cross-cutting	Substitute natural gas	7-9	0.52

The analysis showed a technical maximum potential for future hydrogen demand of 482–534 TWh per year for the German industry. This estimate is based on 2018 production levels and assumes that all technically feasible processes are decarbonised using hydrogen. The potential is driven by the transition to hydrogen-based alternatives for process heating and feedstock use. The basic chemicals and primary steel industries emerge as significant contributors to this hydrogen potential. Together, these two branches have a combined potential of more than 230 TWh/yr in Germany. The spatial distribution and height of the hydrogen demand potential are aggregated per NUTS3 region as visualised in Figure 6a. For example, 24.5% (80 TWh/yr) of this demand is concentrated at only three sites, while the 20 largest sites represent approximately 74% of the identified potentials. The spatial distribution at NUTS3 level obtained in Paper 1 and the site-specific correlation with the natural gas transport network indicate the current dependency on the gas infrastructure

(Fig. 6b). Paper B verifies the observation that especially large and energy-intensive industries such as primary steel and basic chemicals production have access to the gas transport network. By extending the approach to Northwestern Europe within Paper II primary steel and basic chemicals production are confirmed to be the largest and most robust industrial hydrogen demanders. The development of site-specific implementation of hydrogen-based processes in 5-year steps until 2035 is analysed, resulting in a total hydrogen demand of 55 TWh in 2030 for those regions, neglecting economic factors.

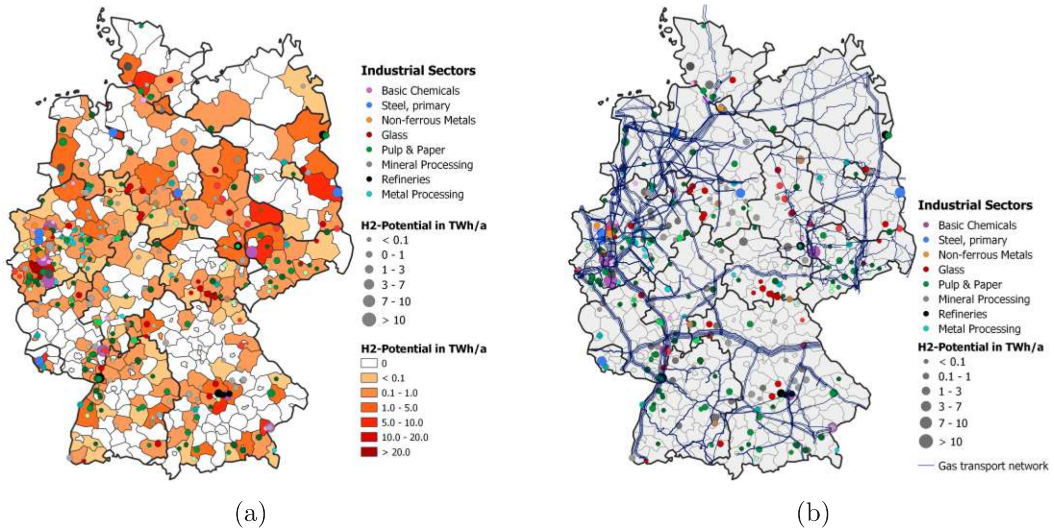


Figure 6: *Spatial distribution of the industry branches and resulting hydrogen demand potential on NUTS3 level (a) and indication of industries‘ dependence on natural gas transport network (b) from Paper 1*
(Source: Neuwirth et al. 2022a)

5.2 Site-specific modelling of the spatial and timely transition

How could the spatial and timely transition towards hydrogen-based processes be captured in energy demand modelling?

The approach, presented in section 4.4 and published in Paper 2, considers existing industry sites and aims to represent the complexities of process diffusion in the industry sector. Implementation of site-specific industry data offers consideration of infrastructure and contributes to closing the gap of detailed spatial results. The results obtained from the models scenarios allow to analyse investment decisions using the current plant age and typical lifetimes as a driver to also include the timely aspects of process diffusion. In its current state, the Fraunhofer ISI IndustrialSiteDatabase, validated in Paper A, provides the essential inputs for energy-intensive industries. The spatial attributes and site-specific properties are coupled and matched with techno-economic data for fossil and hydrogen-based processes. The application of the model in Paper 3 analyses the spatial and timely distribution based on site-specific investment decisions for primary steel, ammonia, methanol and HVC, answering *RQ* 2.1. The transition starts in Northwestern Europe with primary steel and a few ammonia plants reinvesting into hydrogen-based processes until 2030. Towards 2040 the use of hydrogen in these products expands to Eastern and Southern Europe, while investments into hydrogen-based methanol and HVC production develop until 2050 across EU 27+3. The largest hotspot exists in the Antwerp-Rotterdam-Rhine-Ruhr Area (ARRRA) with the highest density of steel and chemical industries in EU27+3. Regarding *RQ* 2.2, the plans for a hydrogen infrastructure according to the EHB initiative are sufficient in most cases to supply the steel and basic chemical sites.

5.3 Sensitivities for hydrogen demand for steel and chemical products

What techno-economic factors determine the diffusion dynamics towards hydrogen-based processes for primary steel and basic chemical production?

In Paper 3, the model from Paper 2 is applied to all European primary steel, ammonia, methanol, and HVC sites. The analysis of reinvestment cycles shows that the complete replacement of the current plant fleet of these products in the EU27+3 is theoretically possible by 2050, but most plants have only one reinvestment cycle left. About 36% of the plants considered (39% in terms of production capacity) need replacement by 2030, and 58% (68% translated to capacity accordingly) by 2035, posing a risk of lock-ins in fossil fuel-based processes as hydrogen-based processes are not yet economically competitive. Those two indicators, plant-specific reinvestment cycles, and economic competitiveness, highly influence the market diffusion of hydrogen-based processes in Paper 3. The calculation of 16 sensitivities, based on four price path variations for hydrogen and CO_2 certificates, respectively, highlights the dependence on economic competitiveness. Higher CO_2 prices and lower hydrogen prices accelerate the adoption of hydrogen-based processes, while high hydrogen prices and low prices for CO_2 certificates delay it. The results of the process diffusion in Figure 7 show the dependence on the price paths of hydrogen and CO_2 certificates, which contributes to *RQ* 3.1 and *RQ* 3.2.

The results indicate that full market diffusion until 2050 is unlikely from a techno-economic perspective, especially for chemical processes with embedded carbon that are not affected by CO_2 pricing. Early reinvestment needs pose the risk of fossil lock-ins, and long process lifetimes often hinder the possibility of a second investment until 2050. Furthermore, the availability of hydrogen infrastructure is crucial for the successful implementation of hydrogen-based processes. The current plans of the EHB initiative for a European hydrogen transport infrastructure seem to fit well to the industries' reinvestment cycles, answering *RQ* 2.2. Regional differences in hydrogen infrastructure also impact the adoption of hydrogen-based processes, with Northwestern Europe leading the transition.

In general, the economic competitiveness of hydrogen-based processes varies by country, with Germany having the highest manufacturing capacity for the investigated products. Break-even points for switching from coal-fired blast furnaces to DRI based on natural gas or hydrogen depend heavily on prices for CO_2 certificates. Hydrogen-based alternatives for methanol and HVC are not expected to be cost-competitive in the medium term, requiring high prices for CO_2 certificates and low hydrogen prices to become viable. Assuming that the structure and spatial distribution of European industry remain similar to those of today, the highest hydrogen demand for the production of primary steel and basic chemicals will be located in the northwest of Europe, including Germany, the Netherlands, and Belgium. The analysis shows that the hydrogen demand in Northwestern Europe could reach 229 TWh by 2050, with a total of 507 TWh in Europe as a whole. These estimates consider plant ages, reinvestment cycles, and optimistic hydrogen price assumptions, but not specific investment plans or governmental subsidies.

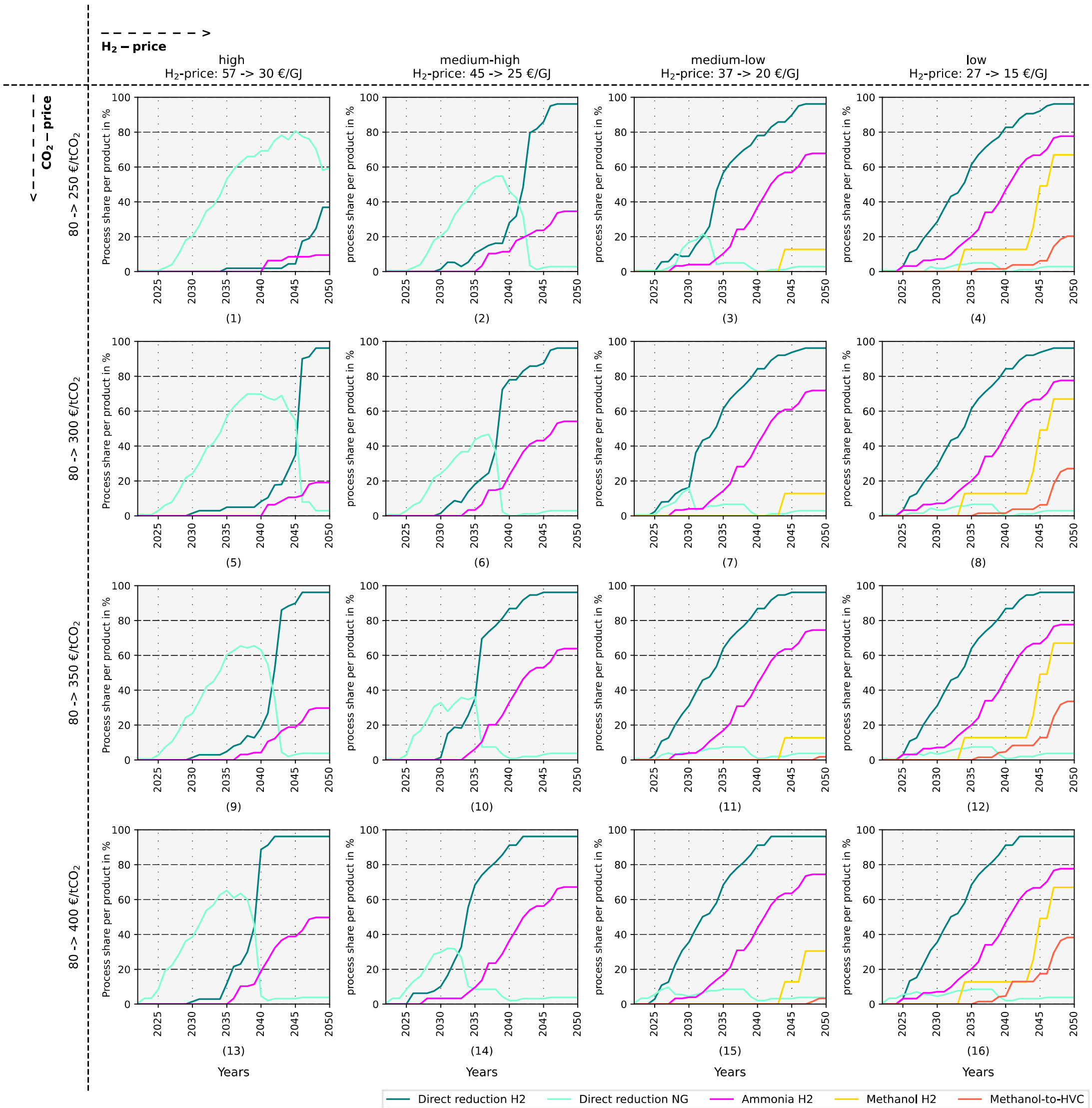


Figure 7: *Share of total production per process depending on hydrogen and CO_2-prices from Paper 3*
(Source: Neuwirth et al. 2024a)

6 Conclusion, critical assessment, and outlook

Decarbonising energy-intensive industries is a big and inevitable challenge to reach climate goals and establish a climate-neutral energy system. Heavy industries account for a huge share of fossil energy demand and face significant technical and economic hurdles in switching to climate-neutral processes (Wesseling et al. 2017). Hydrogen, produced from renewable energy, has the potential to play a key role in the transition towards climate neutrality. In the energy-intensive industry branches, especially primary steel and basic chemicals show the highest and most robust future hydrogen potentials. In addition, current drastic changes within energy systems require robust planning taking into account spatial and temporal dynamics and their interdependencies. Therefore, in this thesis, an individual-level site-specific modelling approach is established to investigate the implementation of hydrogen in the European production of primary steel, ammonia, HVC, and methanol.

The following sections reflect on the scientific contribution and the underlying methodological approach. On the one hand, the TRL and the techno-economic properties of the various hydrogen-based process options were reviewed. On the other hand, the characteristics of individual industry sites, their spatial distribution and the age structure of the current plant stock determine process diffusion in combination with infrastructure access. With reference to the *Key objective* presented in the problem statement in section 3, conclusions are drawn from the results in section 6.1 and critically discussed in section 6.2. Section 6.3 provides an outlook on future research and further improvements.

6.1 Scientific contribution

The two main methodological contributions reflect spatial resolution and consideration of individual plant ages and reinvestment cycles for diffusion dynamics in industry transition pathways. In addition, the developed datasets and methods are provided open source in line with the core publications of this dissertation, including site-specific industry data, hydrogen-based process parameterisation, the site-specific model framework, and analysed scenario results.

Hydrogen contributes to decarbonising the industry sector

Hydrogen is a promising energy carrier that contributes to decarbonising the industry sector. The techno-economic specification of hydrogen-based processes for energy-intensive industries and the corresponding research questions in the context of *RQ* 1 are addressed by a thorough literature research. This results in the analysis of technical hydrogen demand potentials in Germany in Paper 1. A similar approach to the technical assumptions on TRL and the SEC of conventional and alternative process options for energy-intensive industries was published during the course of my thesis by Gailani et al. 2024 and validates the assumptions on hydrogen-based processes from Paper 1. In the steel industry, H2-DRI has the potential to significantly reduce CO_2 emissions. DRI based on natural gas is technically mature, and various German and European projects are announced planning to scale up the use of hydrogen (Verpoort et al. 2024). In the chemical industry, hydrogen also shows great potential, particularly in the production of basic chemicals such as HVC, ammonia, and methanol.

Spatial distribution of hydrogen demand potentials in Germany

Regarding the spatial aspects of *RQ* 2, the resulting site-specific spatial resolution of technical hydrogen demand potentials in Germany in Paper 1 shows that the basic chemicals and primary steel industries emerge as hotspots and significant contributors to industrial hydrogen demand. This high concentration of potential hydrogen demand in a few hotspots highlights the need for strategic infrastructure development. For Germany, regions like North Rhine-Westphalia, Leuna, and Ludwigshafen show a high concentration of potential hydrogen demand. Developing a targeted infrastructure could improve the efficiency and economic viability of hydrogen use in these regions. However, covering the demand potentials apart from those hotspots also entails addressing the spatial disparity in hydrogen demand and establishing a robust distribution network to connect smaller, evenly spread demands. Crucially, realising the entire potential demand necessitates enormous amounts of renewable electricity, which exceeds Germany's total electricity consumption of 500 TWh in 2019 (AGEB 2024). These large numbers indicate the critical need for massive expansion in renewable energy and their respective infrastructure.

Site-specific modelling to improve spatial and timely resolution

Following the goal within *RQ* 2 to not only assess the spatial distribution of hydrogen potentials, but also include a timely transition based on site-specific investment decisions, a new modelling approach was established. The model is published open source according to Paper 2 and enables a site-specific resolution by considering existing industry sites and current plant stock to analyse scenarios for the transformation of the European industry sector. In this thesis, primary steel, ammonia, methanol, and HVC are modelled. However, for further products, detailed data, such as plant age, may be lacking for sites in some branches. Reflecting the current industry structure with high resolution, the model supports strategic decision making by providing detailed insight into the timely and spatial distribution of industry transition. Techno-economic calculations evaluate the respective costs on the basis of which investment decisions are made according to the current plant age and theoretical reinvestment cycles. The results obtained from the modelled scenarios contribute to the answers of *RQ* 2.1 and *RQ* 2.2 by analysing investment decisions, energy demands, possible infrastructure access, and the impact of policies such as CO_2 pricing. The application of the model for all European primary steel, ammonia, HVC, and methanol sites in Paper 3 shows that Northwest Europe has the highest industry density for these branches. The results underscore the importance of spatially targeted infrastructure development and the need for flexible investment strategies. As mentioned above, strategic planning and timely investments in hydrogen infrastructure are crucial to avoiding carbon lock-ins. The current plans of the EHB initiative cover almost all European primary steel and basic chemicals sites sufficiently and also fit well with the timely development of the identified reinvestment needs.

Investigation for primary steel and basic chemicals in EU27+3

The investigation of the process diffusion and the spatial and temporal dynamics for the production of primary steel, ammonia, HVC, and methanol in Paper 3 revealed the critical role of economic frameworks in the influence of investment decisions referring to *RQ* 3. The reinvestment cycles of the existing plant stock and the age distribution indicate that at least one investment opportunity remains until 2050 for most plants, with 36% of the plants considered requiring reinvestment by 2030 and 58% by 2035 (representing 39% and 68% of the European capacity for the considered products, respectively). This early need for reinvestment represents a high risk of lock-ins to fossil fuel-based processes unless competitive climate-neutral alternatives are developed and supported by policies. The spatial and temporal results related to *RQ* 3.1 highlight the need for infrastructures such as the EHB to avoid potential lock-ins. Assuming that the structure and spatial distribution of European industry remain similar to those of today, the highest hydrogen demand for the production of primary steel and basic chemicals will be located in the northwest of Europe, including Germany, the Netherlands, and Belgium. By 2050, the hydrogen demand in Northwestern Europe could reach 229 TWh, with a total of 507 TWh in Europe as a whole, taking into account plant age and reinvestment cycles as well as favourable economic conditions for hydrogen. To understand the impact of different price developments of hydrogen and CO_2 certificates on diffusion dynamics, 16 sensitivities are calculated for varying hydrogen and CO_2 price projections (4 variations each), related to *RQ* 3.2. The results of the process diffusion in Figure 7 clearly show the dependence on the price projections, which are associated with significant uncertainties. The economic viability varies strongly among the products and processes. In other words, hydrogen-based alternatives for methanol and HVCs will likely not be cost-competitive in the medium term and will require low hydrogen prices. Here, the CO_2 price has a particularly weak impact, as most of the carbon is embedded in the products rather than emitted during production (scope 1 emissions). In contrast, for steel, the combination of a high impact of the CO_2 price on coal-fired blast furnaces and the opportunity to use natural gas for NG-DRI as a bridging option to hydrogen helps mitigate the risk of fossil lock-ins.

The most important limitations of this thesis are discussed in the following section 6.2.

6.2 Critical assessment

The dissertation evaluates the dependencies of plant age, lifetimes, and site-specific spatial distribution of energy-intensive industry sites to project process diffusion in industry transition. However, the model approach requires a variety of exogenous input data, and the complex heterogeneous structure of the industry sector enforces simplifications. Therefore, several limitations must be considered when evaluating the results.

The parameterisation of industry processes affects the economic calculations that lead to respective investment decisions within the model. Data for specific investment, specific operational and maintenance costs, specific energy and feedstock consumption, and lifetime are determinants. The reliability of industry site data, especially the plant age, is hard to gather and crucial for the temporal aspect of the process diffusion in the presented model. In reality, other factors also influence the point of time for investment decisions. However, soft indicators that influence individual investment decisions are difficult to quantify, and the approach based on the age and lifetime of the plant improves current implementations and provides a good estimate. So far, the model does not consider specific future investment plans of companies or government subsidies, which are already partially announced.

In general, the ability to model entire process chains depends on data availability and requires enormous process detail. In the current model, each production unit represents an integrated process chain to ensure comparability. More detailed data for the parameterisation of processes are required to model subproduction units and derive more specified results.
However, uncertainties in the description of industrial transition pathways arise not only from industry-related factors. The industry sector also relies on external developments, especially for energy prices, which evolve from overarching social, economic, and geopolitical trends and market mechanisms within the entire energy system. A recent example is the price shocks following the Russian invasion of Ukraine and Europe's dependence on Russian energy imports. The complexity of those incidents cannot be included in such models, especially not in a model that only covers parts of one sector, as presented here. Conducting different scenarios with varying assumptions helps in sensitivity analysis for decisive parameters to draw robust conclusions. However, perfect foresight of the energy price projections and the lack of flexibility options due to the annual resolution mark limits of the approach.

The existence of a hydrogen infrastructure is a prerequisite for the adoption of hydrogen-based processes. The alignment of hydrogen demand with the proposed plans for hydrogen infrastructure from the EHB initiative suggests that most sites will be integrated into the planned network. Furthermore, transport of CO_2, essential for the production of methanol and the MtO route, would be eligible to be considered but are not yet part of the model. However, first attempts were recently published in literature that assess and optimise the options for pipeline routing of future CO_2 pipeline networks using geoinformation systems (GIS) (Yeates et al. 2024).

Within this thesis, only hydrogen-based processes are analysed as alternatives to current fossil production. In addition to hydrogen, other important decarbonisation strategies include the direct electrification of processes, the use of CCU/S (Carbon Capture, Utilisation, and Storage), and biomass. These options were not included in the quantitative modelling but play a crucial role in the future decarbonisation of the industry. The decarbonisation of low- and medium-temperature process heat is likely to be more economical and energy efficient by direct electrification than the use of hydrogen (Fleiter et al. 2024b). In addition, direct electrification of HT processes could be an alternative to hydrogen-based processes, although technically it is not yet mature in most applications (Fleiter et al. 2024b). The current status of the model can only represent existing industry sites provided as model input and evaluates a process switch of those existing facilities. However, instead of substituting and replacing existing plants, new industry sites may arise at currently unknown locations with unknown capacity and processes.

6.3 Outlook

A site- and plant-specific modelling approach was established to assess industry transition pathways in the context of a climate-neutral energy system.

Future work needs to continue on the transition of industry towards climate-neutral processes and the integration into the energy system. Section 6.2 already represents a critical discussion of the model presented and highlights its limitations, on which future work could focus to improve. Given the high uncertainty about the future role of hydrogen in the energy system, further analyses that model the complete energy system can build on results and data of the model developed within this thesis. One major task in further research is to model and plan energy infrastructures aligned with the needs of the demand and supply sectors. Energy system models incorporating such spatially highly resolved data can contribute in strategically guiding required policies. In particular, direct electrification of industrial process heat and the implementation of CCU/S processes under a carbon management strategy will complement the use of hydrogen. Therefore, complementing the present work with more competing processes to assess various decarbonisation pathways and an extension of the approach to all energy-intensive industry sites is a priority for future investigations.

Future model development should consider investment announcements, corporate strategies, and the connection to the electricity grid to investigate more realistic transformation paths. Integrating markets where the individual sites participate would allow to examine an agent behaviour and direct connection between the industries in a more complex system. However, the site-specific resolution of the model and underlying data, both published open source, provide the basis for further development to answer open research questions in different directions. The combination of spatial and timely dynamics of industry transition will be an ongoing process to be assessed. Within this thesis, the investigation of the spatial and temporal dynamics of process diffusion for the production of primary steel, ammonia, HVC, and methanol revealed the critical role of economic frameworks in influencing investment decisions. The reinvestment cycles of existing plants indicate a high risk of lock-ins to fossil fuel-based processes unless competitive climate-neutral alternatives are developed and supported by policies.

Summarised, the transition to hydrogen-based industrial processes presents significant opportunities and challenges. The substantial hydrogen demand potential could contribute to emission reduction in energy-intensive industries but requires extensive renewable electricity generation and the development of strategic infrastructure. However, the realisation of future hydrogen demand depends on many factors, including energy prices, policy measures, and industrial investment decisions. The results show that future hydrogen demand can vary greatly depending on the assumptions and scenarios considered. Site-specific modelling offers a framework for understanding process diffusion and supporting policy decisions, while analysis of reinvestment cycles highlights the urgency of creating an economic environment that favours climate-neutral processes. Future research should focus on improving data quality, integrating alternative decarbonisation strategies, and examining the global implications of changing value chains. Together, these efforts will support a successful transition to a CO_2 neutral industrial sector.

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Publications

This chapter presents the publications constituting this thesis, including the core publications of this thesis – three journal papers – as well as further publications, comprising two main author publications, five co-author publications and other scientific contributions. For each core publication, the full paper, a short summary, my own contribution based on the CRediT taxonomy[1] and the bibliographic reference are provided. The two other main author publications are also fully attached. Co-author publications and other scientific reports and contributions are briefly described and my contribution to them is presented. The publications are not sorted by release date but instead based on this thesis's incremental research approach and thematic chronology.

Core publications

Further publications and other scientific contributions

[1] According to the Elsevier CRediT author statement: https://www.elsevier.com/authors/policies-and-guidelines/credit-author-statement

Paper 1

The future potential hydrogen demand in energy-intensive industries - a site-specific approach applied to Germany

published in Energy Conversion and Management in collaboration with Tobias Fleiter and René Hofmann

This journal paper covers an analysis of hydrogen-based industry production for the energy-intensive branches of iron and steel, non-metallic minerals, basic chemicals, pulp and paper, and refineries in Germany. The paper mainly relates to *RQ* 1 and aims to review the process options in energy-intensive industry branches to switch to hydrogen-based production and to parametrise the specific hydrogen consumption of these options. Based on this literature review, the TRL for the identified processes was estimated. A bottom-up approach helps to analyse the spatial distribution of the future hydrogen potential for the covered industries in Germany. Matching the identified processes and their estimations of specific hydrogen consumption with the established Fraunhofer ISI IndustrialSiteDatabase results in site-specific hydrogen demand potentials for 367 individual industry sites. It was observed that a few hotspots account for the major share of hydrogen potential in Germany. This heterogeneous picture show that many regions will demand relatively small amounts of hydrogen, while a few regions can become major hydrogen demand centers. The spatial results indicate that this very uneven distribution needs to be considered when building a hydrogen transport infrastructure. Complementing the bottom-up approach for the energy-intensive industry branches, a top-down calculation was conducted to estimate the total hydrogen potential and the corresponding emission reduction potential for the entire industry sector. The underlying data is published and visualised as open data in line with this publication on the following website: https://isi.pages.fraunhofer.de/pshp/. The data set can be used to perform a more detailed analysis on the systemic interaction of energy-intensive industry sites with other parts of the energy system and infrastructure. Based on this publication, the current dependency of the respective industry branches on the natural gas transport network in Paper B was analysed. The Papers II, 2, and 3 build on the parametrisation of hydrogen-based processes derived within this publication.

My contribution: Conceptualisation, Methodology, Validation, Investigation, Formal Analysis, Data Curation, Writing - Original Draft & Editing, Visualisation.

M. Neuwirth, T. Fleiter, P. Manz & R. Hofmann (2022a). "The future potential hydrogen demand in energy-intensive industries - a site-specific approach applied to Germany". In: Energy Conversion and Management *252, p. 115052. ISSN: 01968904.*
DOI: `10.1016/j.enconman.2021.115052`

Energy Conversion and Management 252 (2022) 115052

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

The future potential hydrogen demand in energy-intensive industries - a site-specific approach applied to Germany

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ARTICLE INFO

Keywords:
Hydrogen
Demand
Energy-intensive industry
Innovative technologies
Site-specific
Potential
CO_2-neutral industry

ABSTRACT

Hydrogen, when based on renewable electricity, can play a key role in the transition towards CO_2-neutral industrial production, since its use as an energy carrier as well as a feedstock in various industrial process routes is promising. At the same time, a large-scale roll-out of hydrogen for industrial use would entail substantial impacts on the energy system, which can only be assessed if the regional distribution of future hydrogen demand is considered.

Here, we assess the technical potential of hydrogen-based technologies for energy-intensive industries in Germany. The site-specific and process-specific bottom-up calculation considers 615 individual plants at 367 sites, and results in a total potential hydrogen demand of 326 TWh/a. The results are available as an open dataset. Using hydrogen for non-energy-intensive sectors as well increases the potential hydrogen demand to between 482 and 534 TWh/a for Germany - based on today's industrial structure and production output. This assumes that fossil fuels are almost completely replaced by hydrogen for process heating and feedstocks. The resulting hydrogen demand is very unevenly distributed: a few sites account for the majority of the overall potential and, similarly, the bulk of demand is concentrated in a few regions with steel and chemical clusters.

1. Introduction

The German federal government set mitigation targets in the context of passing the national Climate Protection Act in November 2019 and has revised them in 2021 [1]. These include a 65% reduction in greenhouse gas emissions by 2030 compared to the base year 1990 and climate neutrality by 2045 [1]. The industrial sector is one of the largest emitting sectors with approx. 23% of the total GHG emissions in Germany in 2018. It accounts for almost 30% of the country's final energy demand and uses predominantly fossil fuels [2,3]. In particular, energy-intensive sectors such as steel, non-ferrous metals, cement, chemicals, glass, paper and refineries face major challenges when trying to achieve ambitious climate mitigation targets due to their high specific and absolute emissions in combination with technical and economic restrictions that prevent them from switching to low-carbon technologies. The need for very high temperatures (often greater than 1000 °C) and large quantities of energy mostly excludes the direct use of renewable energy sources. In addition, process-related GHG emissions that are inherently related to the production process require completely new designs that are often not yet available or cost-competitive. Industry also uses large amounts of fossil fuels as feedstock.

Consequently, in most industries, substantial change is needed to avoid the use of fossil fuels and carbon-based feedstocks. One solution that is currently being discussed very prominently is the substitution of fossil fuels by hydrogen produced from green electricity. Hydrogen can be used to provide high-temperature process heat and is a potentially

Abbreviations: °C, Temperature in degree Celsius; AGEB, Working Group Energy Balances; BMWi, Federal Ministry for Economic Affairs and Energy; CCfD, Carbon Contract for Difference; CO_2, Carbon dioxide; E-PRTR, European Pollutant Release and Transfer Register; EU ETS, European Union Emission Trading System; GHG, Greenhouse Gas; GJ, Gigajoule; H_2, Hydrogen; H_2-DRI, Direct Reduced Iron using Hydrogen; ISI, Institute for Systems and Innovation Research; Mt, Megaton; MtO, Methanol-to-Olefins; NG, Natural gas; NUTS, Nomenclature of Territorial Units for Statistics; NHS, National Hydrogen Strategy of Germany; R&D, Research & Development; SEC, Specific Energy Consumption; SMR, Steam Methane Reforming; TRL, Technology Readiness Level; TWh, Terawatt hours; VDZ, Association of German cement companies.

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https://doi.org/10.1016/j.enconman.2021.115052
Received 8 September 2021; Received in revised form 7 November 2021; Accepted 20 November 2021
Available online 28 December 2021

CO_2-neutral feedstock for the chemical industry. As a storable medium, hydrogen can also be used directly and indirectly for energy storage to balance fluctuations of renewable energies in the future [4–6].

While there are high hopes that hydrogen can help to decarbonize industry, there is still very high uncertainty about the integration of green hydrogen into the energy system. Unlike other potentially CO_2-neutral energy carriers like electricity or clean gas, there is currently virtually no generation capacity or transport infrastructure available for green hydrogen. The large-scale use of hydrogen would require the construction of infrastructure, which is already under research [7], and generation capacity and induce major changes in the energy system with potentially high costs [8]. As water electrolysis is expected to be the main supplier of hydrogen in the future, it is clear that the implementation of alternative technologies is only reasonable if a sufficient supply of renewable electricity can be guaranteed.

In 2020, the German government set targets for the use of green hydrogen in its national hydrogen strategy (NHS) [9]. The aim of the national hydrogen strategy is to leverage the potential of hydrogen technologies and bring about a real market ramp-up together with the economy by creating the framework to make hydrogen competitive and attractive for investments in its economic and sustainable production, transport and use. To reach these goals, pilot programs for Carbon Contracts for Difference (CCfD) and international solutions for markets of climate-neutral products are planned. In the long term, hydrogen is therefore seen as having an important role in securing Germany's position as an industrial player [9]. In order to better understand the integration of hydrogen and the transition of the energy and industrial systems, it is first necessary to obtain a clear picture of the potential hydrogen demand of industry as well as detailed knowledge about the spatial distribution of the demand for future developments. This includes the overall potential quantity, but also the locations as well as the technological maturity.

This paper presents a first approach for estimating site-specific potentials of hydrogen-based processes.

Several studies have recently become available that aim at estimating industry's potential future hydrogen demand. However, these studies generally have a narrow scope with a technology-specific, sectoral or strongly limited regional focus. Studies with a broader scope that include several industries and processes mostly report hydrogen potentials on aggregated sectoral and regional levels and often only for applications where hydrogen can be used as feedstock. Agora (2019) [10] investigated possible technology options for the decarbonization of basic chemicals, steel and cement, and considered hydrogen use as a feedstock for basic chemicals and for direct reduction of iron ore (H_2-DRI) for steel industry. Dechema (2017 & 2019) [11,12] as well as Stork et al. (2018) [13] focused on low-carbon energy and feedstock possibilities for the chemical industry and highlighted the most important techno-economic parameters by developing roadmaps towards 2050. Numerous other research publications are available that address individual products and processes for the manufacturing of ammonia [14–22], methanol [23–29], olefins [30–32] and steel [33–38] by using hydrogen from different sources. Further studies outlining the ways to decarbonize selected industries include, for instance, Prognos (2020) [39] for refineries, VDZ 2020 [40] for cement, and Ireson et al. (2019) [41] and Glass Alliance Europe (2019) [42] for the glass industry. In contrast, other research in the field of energy system analysis focuses on decarbonization scenarios at regional or country level, such as ISI [43] and Dena (2018) [44]. To conclude, currently, no comprehensive estimation of site-specific hydrogen potentials is available.

We aim to close this research gap by providing a methodology to estimate the potential hydrogen demand of industry including comprehensive open source data with site-specific results for Germany. In doing so, we focus entirely on the demand for hydrogen, and exclude supply-related questions. Here, we refer to other already available research on hydrogen supply technologies like steam methane reforming and water electrolysis and their corresponding costs [45–53]. Our focus is on the processes of energy-intensive industry. This includes the use of hydrogen as a feedstock for the production of, e.g. ammonia, methanol, and ethylene, as well as the energetic use of hydrogen in high-temperature furnaces and steam generators across industry sectors. This leads to the following main research question:

What is the maximum potential future demand for hydrogen in energy-intensive industries and how is this spatially distributed?

We aim to address this research question from a bottom-up perspective by identifying relevant individual production processes and reviewing the technology options to decarbonize them using hydrogen. To assess the spatial distribution of hydrogen demand, we compiled a site-specific dataset for all relevant energy-intensive industries in Germany. Site and process-specific information like type of process and knowledge about the industrial plant stock provides the basis for calculating the process-specific potential hydrogen demand. The focus of our research is on the development of this dataset and the review of technologies' parameters and maturity.

Our aim is not, however, to forecast hydrogen demand. Instead, we propose a transparent method and apply it to calculate the technical potential of hydrogen demand. Both the resulting dataset and the method can be used in further studies to develop more specific hydrogen-use scenarios towards 2030 or 2045/2050.

The resulting dataset covers the following dimensions:

- **Site-specific information:** Industrial subsector and conventional processes together with the number of corresponding plants and production volumes as well as the alternative hydrogen-based production processes.
- **Spatial information:** Geoinformation for all industrial sites (geocoordinates).
- **Process-specific information:** Process-specific information such as the specific energy consumption and market maturity of conventional and possible new, alternative hydrogen-based technologies.

To summarize, we estimate the process-specific and site-specific potential hydrogen demand from using hydrogen-based production technologies. Further, we provide an open dataset[1] with detailed site-specific and process-specific information with the calculated maximum potentials of future hydrogen demand.

Section 2 presents the method and data needed to calculate the resulting hydrogen demand potentials. Section 3 shows the detailed analysis and presentation of the findings merged at different sectoral and regional levels and key findings are discussed in section 4. Finally, conclusions are derived in section 5.

2. Methodology and data

Our method is based on a comprehensive bottom-up calculation of site-specific and process-specific technologies of energy-intensive industries, which account for about 75% of the energy use in industry in Germany [54]. The approach consists of the three following major steps:

1. **Estimation of process-specific hydrogen demand potentials:** We estimate potential hydrogen demand assuming that the main processes in energy-intensive industries switch to hydrogen as a fuel and as a feedstock. The estimation depends on the respective specific energy consumption of the identified hydrogen-based process technologies and is related to the physical production output (unit: GJ/t product output). The potentials are calculated independently of geographical context, but with specific knowledge of the industrial process involved. Therefore, a comprehensive literature review was

[1] Please cite and refer to this publication when using the dataset. Visualization and download of the licensed data is available under: https://isi.pages.fraunhofer.de/pshp/

Table 1
Overview of production processes in the scope of our analysis with production output and fossil energy demand of 2018.

Industrial subsector	Process/Product	Production output in Mt	Fossil energy demand in TWh/a	Source
Iron and steel	Crude steel, primary	29.6	97	[54]
Basic Chemicals	Ammonia	2.9	26.2	[55]
	Methanol	1.1	11.5	[55]
	Ethylene	4.7	47.9	[55]
	Other olefins	4.7		[55]
Refineries	Oil products	131.8	61.5	[56]
Non-ferrous metals	Aluminum, primary	0.53	4	[57]
Metal processing	Casting	42.0	1.2	[58]
	Rolling, hot	36.6	18.5	[58]
Non-metallic minerals	Container glass	4.1	6.6	[59]
	Flat glass	2.2	5.6	[59]
	Ceramics	14.1	9	[60]
	Cement / Clinker	24.5	11.8	[61]
	Lime burning	6.4		[60]
Paper and printing	Board & Packaging paper	12	16.3	[62]
	Tissue paper	1.5	2.9	[62]
	Graphic paper	7.7	15.4	[62]
	Recovered Fibers	17.2	2.6	[62]
	Chemical pulp	1.4	4.8	[62]

carried out to collect information about technologies and specific processes.

2. **Development of a dataset of industrial sites and plants:** The dataset consists of the major plants in energy-intensive industries and contains information on the relevant processes and the annual production output of main industrial bulk products, among others. This dataset is constructed by combining several individual datasets on emissions reporting as well as sectoral asset information.
3. **Allocation of process-specific hydrogen potentials to sites and plants:** The specific hydrogen potentials per process resulting from step 1 are matched with the dataset from step 2 and calculated per plant.

The site-specific analysis is then supplemented by a top-down estimation of the potential hydrogen demand in the remaining industries, for which no site-specific information was available (see section 3.2). These are mainly non-energy-intensive sectors and including them allows us to develop a complete picture of the hydrogen demand in the entire industry sector. The top-down estimation is based on energy balances.

The following subsections present the successive steps needed to calculate the site-specific hydrogen demand potentials, each with the respective reviewed data and method.

2.1. Estimation of process-specific hydrogen potentials

First, the methodological approach is described in more detail before the energy-intensive industrial subsectors are specified with conventional and alternative hydrogen-based processes. The respective parameters, such as specific energy consumption and production output, were collected by reviewing the literature for both conventional production and hydrogen-based decarbonization options. The most important key aspects and parameters are summarized below. Extensive technology descriptions for each subsector are shown in **appendix B**.

2.1.1. Methodological approach for estimating process-specific potentials

We investigated the technical feasibility of switching from today's mostly fossil fuel-based production processes to hydrogen-based alternatives and estimated the resulting potential hydrogen demand on a process level. Production processes which currently use fossil-based hydrogen were also included in the analysis and the potential demand for (green) hydrogen is calculated. To quantify hydrogen demand potentials, the following information is gathered for each process type:

- Current state-of-the art processes and hydrogen-based alternatives which are currently under investigation in numerous research projects and discussed in the community of energy systems analysis.
- The technology readiness level (TRL) helps to evaluate the status of the technologies. This provides an indicator about the status of development and the remaining effort required until market readiness. This also enables a transparent comparison of several different technologies.
- Specific energy consumption (SEC) represents the energy use of the individual process per ton of product output. We distinguish fuel and feedstock use and exclude electricity, as we only consider the potential for hydrogen to replace fossil energy carriers.
- Temperature level of the process: Due to the combustion properties of hydrogen (high temperatures), replacing fossil fuels by hydrogen in the future to provide process heat seems much more feasible where high-temperature process heat is required.
- Annual production output: We use the production output to calculate capacity utilization factors for each process/product as a basis for the allocation to individual plants (see section 2.2).

In the following, we discuss the feasibility of using hydrogen in the most important industrial processes based on a review of the relevant literature. We briefly describe the technologies used today and discuss the applicability of hydrogen-based alternatives in **appendix B**.

Table 1 summarizes the national production output and fossil energy demand for 2018. The specific energy consumption and process temperature, as well as the expected TRL are shown in Table 2.

2.1.2. Summarized data for estimating process-specific hydrogen potentials

Table 1 shows the identified technologies for future hydrogen potentials from the bottom-up approach with the production volumes and fossil fuel demand based on 2018 figures. Where hydrogen is used as a feedstock for the production of ammonia and methanol in the chemical industry, only changes in the technologies supplying hydrogen have to be made for decarbonization. The additional external hydrogen demand for crude oil refining in refineries also shows potential for substitution with climate-neutral hydrogen. Further efforts and investments are needed for H_2-DRI plants in the steel industry and methanol-based olefin production. Here, the capacities for methanol processing must increase enormously (by a factor of about 17) and new plants for methanol-to-olefins synthesis must be built to meet the high demand for methanol.

In the industrial processes where hydrogen shows potential for supplying process heat, conventional burners can be partly further operated during the transition period using low admixtures of hydrogen

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Table 2
Process-specific energy consumption data to identify the hydrogen potential per process

Process	Technology	Process temperature (°C)	Fuel SEC (MWh/t)	Feedstock SEC (MWh/t)	TRL (1–9)	Source
Iron and steel						
Crude steel, primary	*Blast furnace*	1200–1450	3.2	–	9	[63,64]
	H_2-DRI		–	1.89	8	[34,36,37]
Metal processing						
Casting	*NG burner*	1100–1600	0.008	–	9	[64]
			0.028			[35]
	H_2-burner for process heat		0.028	–	4–5	
Rolling (hot)	*NG burner*	700–1250	0.67	–	9	[35,63]
			0.58-0.61			[34,35,64]
			0.35			[65]
	H_2-burner for process heat		0.67	–	4–5	
Non-ferrous metals						
Aluminum, primary	*NG burner*	700–950	2.1	–	9	[63]
			2.2			[35]
			Melting: 1.3			[66]
			Casting: 0.6			[66]
	H_2-burner for process heat		1.9	–	4–5	
Glass						
Container glass*Recuperative*	*NG burner*	1450–1650	1.61	–	9	[63,67]
			1.28-1.72			[68]
	H_2-burner in furnace	1450–1650	1.28	–	4–5	
Flat glass*Recuperative*	*NG burner*	1450–1650	3.03	–	9	[63,69]
			2.17-2.56			[68]
			2.58			[67]
	H_2-burner in furnace	1450–1650	2.17	–	4–5	
Mineral processing						
Cement/Clinker	*NG burner*	1400–1450	0.97	–	9	[63]
			0.83-1.25			[68]
			1.08			[70]
	H_2-burner in rotary kiln	1400–1450	0.97	–	4–5	
Lime burning	*NG burner*	900–1200	1.03	–	9	[63,69]
			1.14			[70]
	H_2-burner in furnace	900–1200	1.03	–	3–5	
Pulp and paper						
Board & packaging paper	*NG burner*	80–220	1.36	–	9	[69]
			1.36-1.58			[68]
	H_2-burner in steam generator	80–220	1.36	–	8–9	
Tissue paper	*NG burner*	80–220	1.92	–	9	[69]
			1.92-2.25			[68]
	H_2-burner in steam generator	80–220	1.92	–	8–9	
Graphic paper	*Ng burner*	80–220	2.0	–	9	[69]
			2.0-2.33			[68]
	H_2-burner in steam generator	80–220	2.0	–	8–9	
Recovered Fibers	*NG burner*	80–220	0.139	–	9	[69]
			0.139-0.167			[67,68]
	H_2-burner in steam generator	80–220	0.15	–	8–9	
Chemical pulp	*NG burner*	130–150	3.42	–	9	[69]
			2.86-3.42			[68]
	H_2-burner for process heat	130–150	2.86	–	8–9	
Basic chemicals						
Olefins	*Steam cracker*	800–950	Furnace 6.64	–	9	[64,68,70]
			Boiler: 3.17-3.69			
	Methanol-to-Olefins		–	17.67	8–9	[72]
Methanol	*H_2 from steam reforming*	200–300	4.17	6.31	9	[64,70]
	H_2 from electrolysis		–	6.31	8–9	[72]
Ammonia	*Steam reforming*	350–550	3.14	5.92	9	[64,70]
			2.5-4.61			[120]
	H_2 from electrolysis		–	5.92	9	[72]
Chlorine diaphragm	*NG burner*		0.86	–	9	[64]
			0.81-1.6			[69]
	H_2-burner for process heat		0.86	–	8–9	
Chlorine membrane	*NG burner for process heat*		0.28–0.33	–	9	[64,69]
	H_2-burner for process heat		0.28	–	8–9	
Refineries						
Refinery	*H_2 for crude oil refining*		–	0.389–0.639	9	[69]
	H_2 from electrolysis for hydrotreating		–	–	7–9	

to natural gas in the gas grids. When switching to pure hydrogen, however, investments in new burner technologies are necessary. Overall, 8 industrial subsectors with 19 processes were identified with possible potentials for hydrogen-based technologies. Of these, 5 processes use hydrogen as a feedstock.

Table 2 lists process-specific data on energy consumption (SEC) for conventional and alternative hydrogen-based processes to further estimate future plant-specific hydrogen potentials. For processes where hydrogen is used as a feedstock, the feedstock SEC-values shown represent the amount of hydrogen needed. The fuel SEC values represent the energy demand for the production processes apart from feedstock use. For every application where the energetic use of hydrogen could

Table 3
Overview of used datasets and information included (adapted from [73])

Subsector	Source of sectoral data	Production/ capacity	Location	Processes included
All	European Emission Trading System (EU ETS)	–	Coordinates	Type of process
All	European Pollutant Release and Transfer Register (E-PRTR)	–	Coordinates	Type of process
Iron & steel	VDEh Steel PlantFacts	Annual capacity	City	Primary and secondary steel production, Metal processing, age of installations
Cement/ clinker	Global Cement Directory	Annual capacity	City	Clinker: wet/ dryNumber of kilns
Glass	glassglobal plants	Annual and daily production	Address	Flat, container and tableware glass types together with the type of furnaces
Pulp & paper	RISI Pulp and Paper: Fastmarkets RISI	Annual production	Coordinates	Detailed list of paper grades and produced products
Chlorine	Eurochlor Chlorine Industry Review	Annual capacity	–	Chlorine production by membrane, diaphragm, mercury and other processes
Several	Internet research for individual companies in the EU for ethylene, ammonia, aluminum, petrochemicals, lime burning	Depending on source; annual capacity/ annual production	Depending on source; mostly address	Production processes and type of refinery

contribute to decarbonization, it is assumed that the energy provided by fossil fuels to generate process heat is substituted with hydrogen and that this does not result in major changes compared to the conventional SEC values. However, due to the assumed higher efficiencies of hydrogen combustion, the value for the fuel SEC for the alternative processes is assumed to be at the lower end of the range for conventional technologies.

2.2. Develoment of a dataset of industrial sites and plants

In order to calculate site-specific hydrogen demand potentials, we used the Fraunhofer ISI Industrial Site Database. We supplemented this with additional sites and updates of already existing entries for Germany. The data required concern the relevant plants with information about the industrial subsector, its processes and products as well as the annual production per process.

The used database was originally created by Manz et al. (2018) [72] based on a combination of several different datasets and further developed. For a detailed description of the method, we refer to Manz et al. (2018) [72] and Manz et al. (2021) [73]. In the following, we briefly describe the data included.

Each data entry for an industrial site contains the name of the company and site, the geographical location, the industrial subsector as well as process-specific data for each associated plant such as type of manufactured goods and corresponding production process, annual production and production capacity. The geographical allocation of most industrial sites is mapped using coordinates and, if necessary, its address.

Table 4
Resulting hydrogen potentials in the energy-intensive industries in Germany per subsector and process

Subsector	Number of sites	Number of plants	Potential future H_2 demand in TWh/a	H_2 use in 2018 in TWh/a
Iron and steel	41	132	75	–
Crude Steel, primary	8	16	56	–
Metal processing	30	89	18	–
Casting	24	48	0.8	–
Rolling	16	41	17.2	–
Non-ferrous metals	**4**	**4**	**3.7**	–
Aluminum, primary	4	4	3.7	–
Non-metallic minerals	**130**	**131**	**39.1**	
Glass	**46**	**47**	**8.4**	–
Container glass	33	34	3.6	–
Flat glass	13	13	4.8	–
Mineral processing	**84**	**84**	**30.7**	–
Cement/clinker	32	32	24.0	–
Lime burning	52	52	6.7	–
Pulp and paper	**162**	**322**	**30.5**	–
Board & packaging paper	91	130	10.3	–
Graphic paper	45	50	13.0	–
Tissue paper	17	26	1.9	–
Chemical pulp	6	6	3.3	–
Recovered fibers	83	110	2.0	–
Basic chemicals	**30**	**35**	**161**	18.7
Olefins	9	9	135.5	–
Ammonia	4	4	17	16.9
Methanol	4	4	7	1.8
Chlorine	18	21	1.5	–
Refineries	**16**	**16**	**17.5**	22.7
Total	**367**	**615**	**326**	**41.4**

The Industrial Site Database covers industrial subsectors of the basic material industry such as iron and steel, non-ferrous metals (aluminum), non-metallic minerals (glass) and mineral processing (cement), basic chemicals (olefins, ammonia, methanol and chlorine), pulp and paper, and refineries. These industrial subsectors account for about 75% of the total industrial energy demand [74] in Germany.

Table 3 is a summary of the data sources used to generate the Industrial Site Database. The sectoral asset datasets used for this study originate from various, mostly commercial datasets. These datasets are matched to emission databases (European Emission Trading System (EU ETS)) and the European Pollutant Release and Transfer Register (E-PRTR)) to obtain a single dataset that comprises all the information available about the listed industrial sites together with all the associated processes at one site.

Table 4 shows the previously defined industrial subsectors together with the number of identified sites and plants. For Germany, the final database consists of 367 industrial sites listing information about 615 plants. The spatial distribution of the 367 identified sites with relevant processes is shown in Fig. 1. It can be seen that only a few sites are located in northern regions, while industrial clusters are largely located in west and south-west Germany. More specifically, primary steel production (8), primary aluminum production (4), crude oil refining in refineries (16) as well as the basic chemicals ammonia (4), methanol (4) and olefins (9) are located at a few integrated large-scale manufacturing sites. In contrast, production in other subsectors in Germany is spread across many smaller sites.

Allocation of process-specific hydrogen potentials to sites and plants

To calculate the plant-specific and site-specific hydrogen potentials,

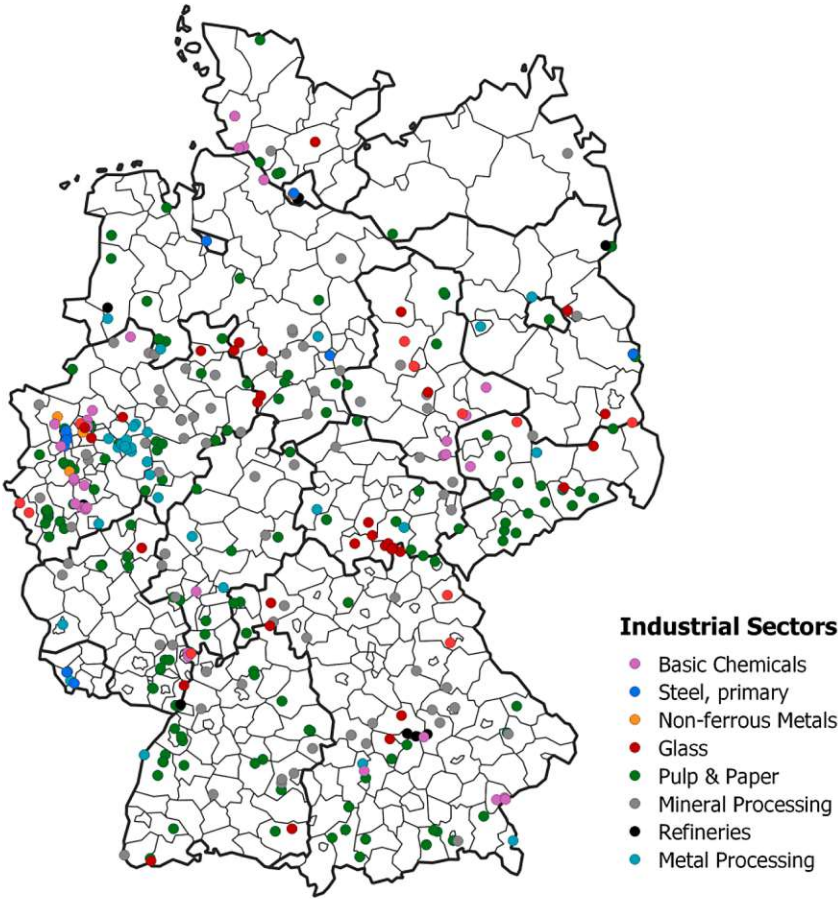

Fig. 1. Identified sites with potential for hydrogen technologies differentiated by industrial subsector.

we match the information gathered in section 2.1 and section 2.2 considering the specific processes of each site. At a site-level, the database only provides production capacities of individual plants. These are translated to the actual estimated production output of 2018 by multiplying with capacity utilization factors from the national German average. Further, SEC-values for hydrogen per process from section 2.1 are assigned to the sites and plants. This method finally leads to equation (1).

$$H_{2,potential,plant} = SEC_{H2,process} \bullet \mathrm{ProdCap}_{\mathrm{plant}} \bullet \frac{\mathrm{Prod}_{\mathrm{process},2018}}{\sum \mathrm{ProdCap}_{\mathrm{process}}} \quad (1)$$

$H_{2,potential,plant}$ is the calculated hydrogen demand potential of the analyzed plant, $SEC_{H2,process}$ the previously identified SEC for the alternative hydrogen-based process, $\frac{Prod_{process,2018}}{\sum ProdCap_{process}}$ the average capacity utilization per process at national level calculated as the quotient of the annual national production output ($Prod_{process,2018}$) and the sum of the capacities of all analyzed plants ($\sum ProdCap_{process}$). This approach assumes that all plants of a certain production process have the same capacity utilization factor and the same SEC. This simplification needs to be considered when using the results of our research. Note that we calculate the technical potential hydrogen demand. This approach is not a forecast, it does not consider any changes in the production volumes of the respective products and plants nor any alternative decarbonization strategies via e.g. switching to secondary processes or using electricity for process heating.

3. Results

The presented results below are supplemented by an open source dataset with detailed site-specific and process-specific information including the resulting hydrogen demand potentials for further research.

3.1. *Site-specific and process-specific hyddrogen potentials (bottom-up approach)*

3.1.1. *Process-specific hydrogen potentials per subsector*

The overall hydrogen demand potential per subsector and process is summarized in Table 4 and corresponds to Fig. 2, which shows the spatial distribution per subsector. It can be seen that around 39.5 TWh/a of hydrogen are already used for manufacturing in the processes considered. Currently, 22.7 TWh/a hydrogen are used in refineries for crude oil refining and methanol production, which is integrated in 3 refineries. This is why only one site is not integrated in refineries and accounts for 1.8 TWh/a. Ammonia is produced in 4 large-scale plants, with about 17 TWh/a of annual hydrogen demand.

For the investigated industries, 615 individual plants were considered, which add up to a total of 326 TWh/a of possible hydrogen demand. Results for the individual subsectors and processes are shown below.

For **basic chemicals** (Fig. 2 (a)), around 17 TWh/a and 7 TWh/a refer to the production of ammonia and methanol at 4 plants, respectively. Switching olefin production to the very energy-intensive and hydrogen-intensive methanol-to-olefins production route accounts for around 135.5 TWh/a additional hydrogen demand at 9 sites. Chlorine

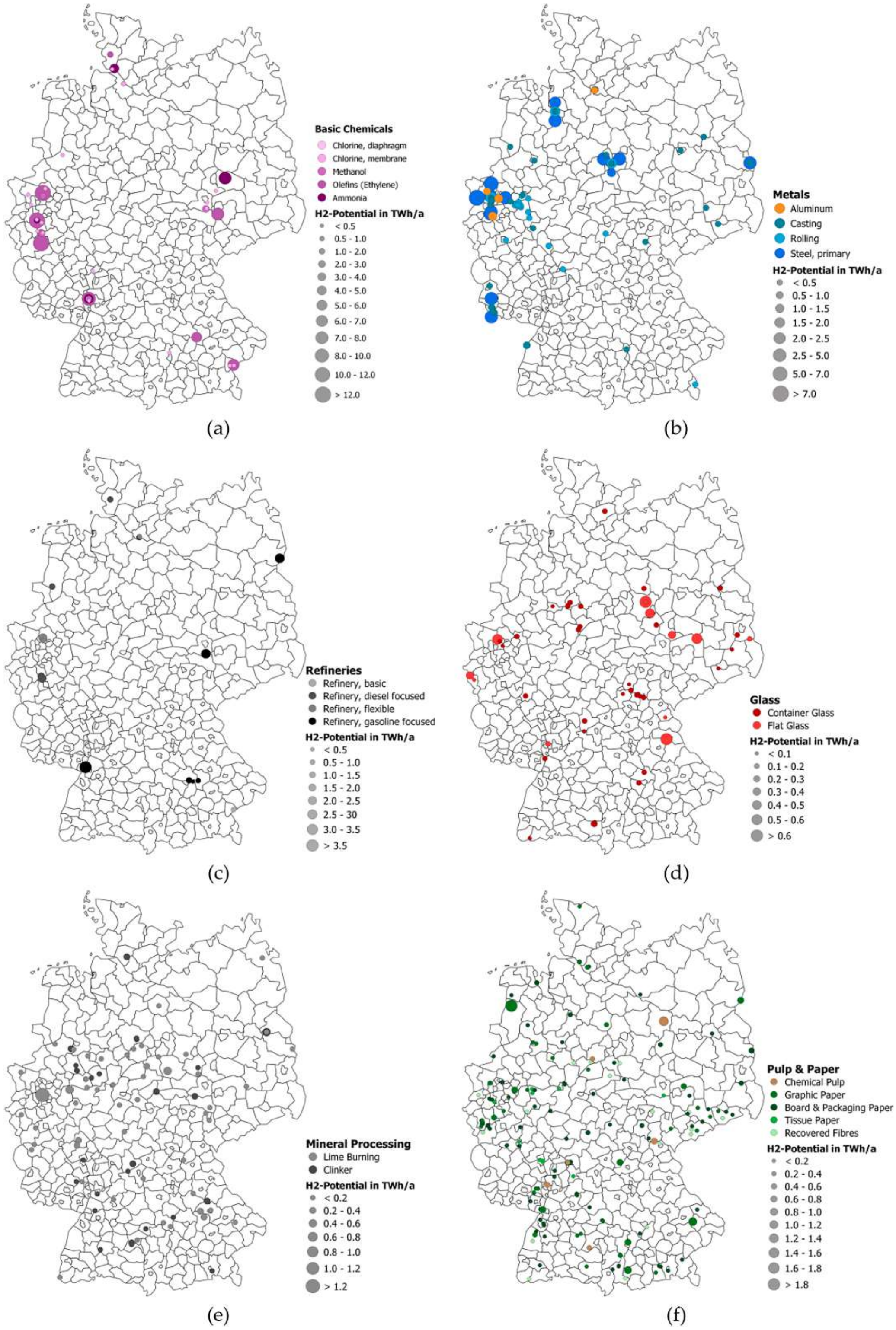

Fig. 2. Spatial distribution of process-specific and plant-specific hydrogen potentials by subsector: (a) basic chemicals; (b) metals; (c) refineries; (d) non-metallic minerals; (e) mineral processing; (f) pulp and paper.

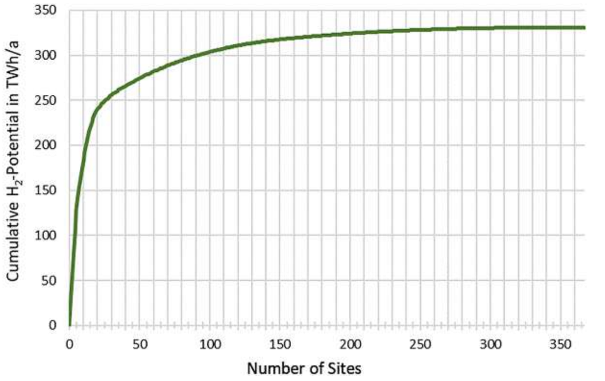

Fig. 3. Cumulative hydrogen demand potential for all identified sites of the energy-intensive industries sorted by size of site-specific potential.

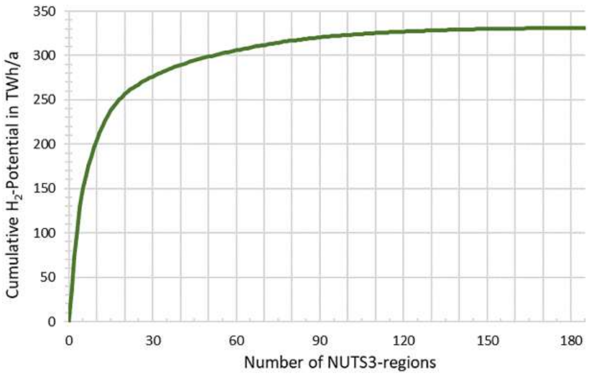

Fig. 4. Cumulative hydrogen potential for all NUTS3 regions with identified hydrogen potential of the energy-intensive industries sorted by size.

has a lower potential with 1.5 TWh/a, accounting for about 0.7 TWh/a for the diaphragm process and 0.8 TWh/a for the membrane process.

Primary crude steel production (Fig. 2 (b)) is located at 8 sites containing 16 plants. Substitution with H_2-DRI results in a potential hydrogen demand of around 56 TWh/a. **Metal processing** is split into casting and rolling (hot). The more energy-intensive process with a higher potential for future hydrogen use is hot rolling in 41 plants and accounts for 17.2 TWh/a. Casting is done at 48 plants and could account for 0.8 TWh/a in total.

For **non-ferrous metals**, site-specific data could be only identified for primary aluminum manufacturing. Here, the 4 production sites in Germany show potential total hydrogen use of about 4 TWh/a, while there is certainly also potential hydrogen demand in the secondary production and in the further processing of non-metallic minerals like aluminum and copper.

The 15 existing **refineries** (Fig. 2 (c)) in Germany together show a hydrogen-demand potential of 17.5 TWh/a. Here, methanol production is not included and fully allocated to the basic chemicals sector.

In the subsector of **glass** manufacturing, companies were split by their products: container and flat glass (Fig. 2 (d)). Overall, of the 47 glass plants, 13 produce flat glass with a potential hydrogen demand of 4.8 TWh/a and 34 container glass companies account for 3.6 TWh/a by switching to hydrogen-fired melting furnaces. Larger hydrogen demand potentials occur for flat glass, as production output is higher for these sites.

The **mineral processing** of clinker production (32 Sites) and lime burning (52 Sites) is presented in (Fig. 2 (e)) with a hydrogen demand potential of 24.0 TWh/a for clinker and 6.7 TWh/a for lime. For both the spatial distribution is spread widely.

The highest number of sites are allocated to the **pulp & paper** industry (Fig. 2 (f)) and differentiated into graphic paper (50 sites, 13.0 TWh/a), tissue paper (26 sites, 1.9 TWh/a), board & packaging paper (130 sites, 10.3 TWh/a), recovered fibers (109 sites, 2.0 TWh/a) and chemical pulp (6 sites, 3.3 TWh/a). This large number of sites is quite evenly spread across Germany without showing hotspot regions per product. The potential hydrogen demand in pulp & paper industry arises from switching to hydrogen-based steam generation for drying and process heat in pulp production.

Fig. 3 presents the cumulative hydrogen demand potential for the industrial sites sorted by size. Here, it becomes obvious that only a few sites account for the majority of the overall site-specific potential. Only 3 sites account for about 80 TWh/a, equaling 24.5% of the total potential, and 7 sites together have a potential of 150 TWh/a. With 240 TWh/a, the largest 20 sites represent about 74% and the largest 50 sites about 84% (274 TWh/a) of the identified potential, and mostly refer to the production of basic chemicals and primary steel. On the other hand, the smallest 100 sites only add up to a potential of about 2 TWh/a, equaling about 0.6% of the total potential; the smallest 150 sites show a potential demand of 5 TWh/a (1.5% of the total potential).

3.1.2. Regional distribution of identified hydrogen potentials in Germany

This section presents the detailed hydrogen potentials at different regional resolutions. Aggregating the site and process-specific potentials results in the spatial distribution at NUTS3 level presented in Fig. 5 (a) and the more aggregated analysis at NUTS1 level (Fig. 5 (b)), which represents the federal states in Germany.

In total, 184 of the 401 NUTS3 regions in Germany show potential future hydrogen demand from the processes and plants considered, with a few, but very big hotspots. 48 NUTS3 regions have low potential up to 0.1 TWh/a. Slightly higher potentials up to 1 TWh/a are distributed over 93 regions, and 28 regions have up to 5 TWh/a. Higher values between 5 and 10 TWh/a are found in 7 regions, and 8 regions have a potential of more than 10 TWh/a, of which 4 could have a future hydrogen demand of 20 TWh/a and higher, up to a maximum of 36 TWh/a in two single NUTS3 regions. Together, these 15 regions that have a hydrogen demand potential of more than 5 TWh/a account for a total potential hydrogen demand of 238 TWh/a, which represents 73% of the total identified potential shown in Fig. 4. These results indicate a very heterogeneous picture for the spatial distribution of Germany's potential hydrogen demand in industry. While some regions can become major hydrogen demand centers, others will hardly demand any hydrogen.

Fig. 5 (b) shows the regional spread at NUTS1 level (federal states). North Rhine-Westphalia has by far the highest future potential, accounting for 145.7 TWh/a, whereas Berlin and Mecklenburg - West Pomerania show nearly no potential for future hydrogen use in energy-intensive industries. Quite low potentials are also observed in central Germany in the federal states of Thuringia and Hessen, with 2.3 TWh/a and 2.6 TWh/a, respectively. This pattern is largely due to the potentially very hydrogen-intensive plants of the chemical and steel industry, which are located to a large extent in North Rhine-Westphalia.

Altogether, Fig. 6 (a) shows a final visualization including all the information for all plants and processes considered together with regional distribution at NUTS3 level.

In total, the regional distribution of the hydrogen demand shows both a high concentration in a few regions and a broad regional spread. 149 regions with low hydrogen potential $<$1 TWh/a are relatively evenly spread across Germany. On the other hand, there are 15 regions with a potential higher than 5 TWh/a. Four of them are located in North Rhine-Westphalia. These are also the regions with the highest potentials including nearly 130 TWh/a for the production of primary steel and basic chemicals. There is an additional hotspot in eastern Germany with a hydrogen potential of 26.5 TWh/a, covering the NUTS3 regions around the refinery in Leuna due to the manufacturing of basic chemicals located there. There are other additional single sites and regions,

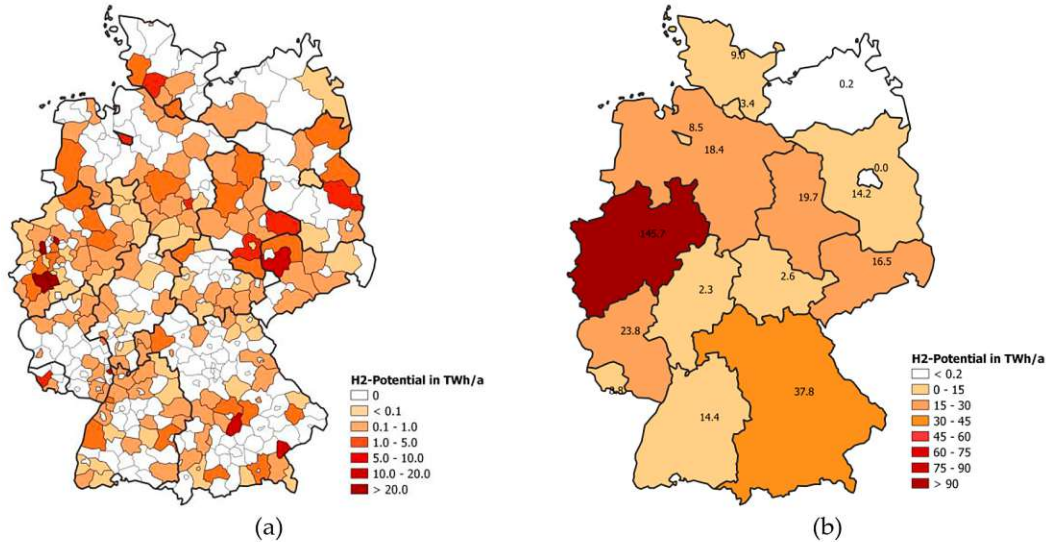

Fig. 5. Identified hydrogen demand potentials in Germany: (a) per NUTS3 region based on process-specific calculations (left); (b) spatial distribution of the hydrogen potentials at the level of the federal states (NUTS1 regions) in Germany (right).

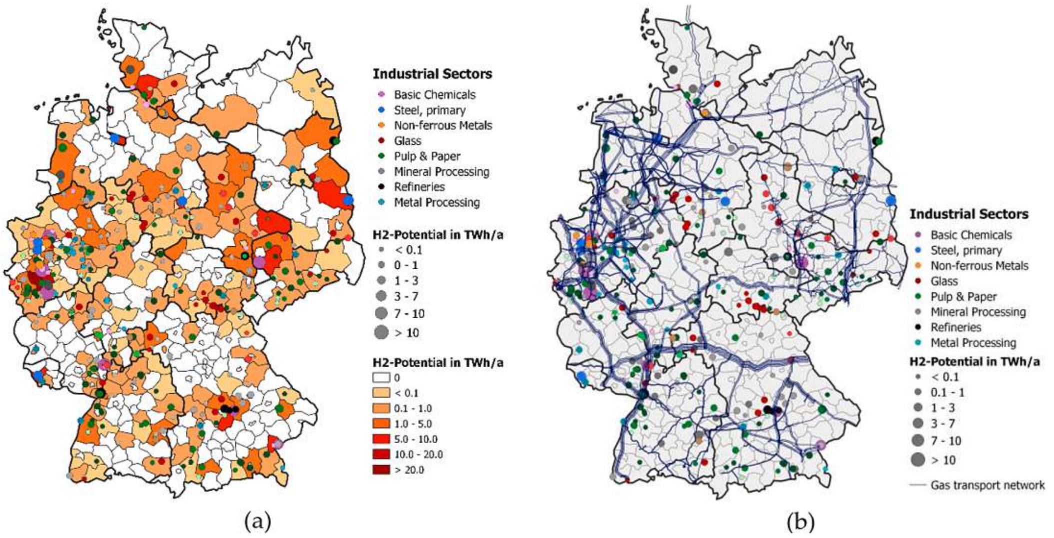

Fig. 6. Site-specific hydrogen potentials for all investigated industrial subsectors and (a) corresponding aggregated demand per NUTS3 region and (b) current natural gas transport network.

like the chemical industry in Ludwigshafen (20 TWh/a), primary steel production in the Saarland (8 TWh/a) and eastern Germany, ammonia production in Brunsbüttel in northern Germany, and olefin production at refineries in Bavaria.

Any plans made for the uptake of hydrogen transport and supply infrastructure need to consider these potential hotspots - primarily in North Rhine-Westphalia. A relatively small hydrogen transport infrastructure would be sufficient to connect, for example, 175 TWh/a of demand located at the three major demand centers in North Rhine-Westphalia, Leuna and Ludwigshafen. On the other hand, substantially larger infrastructure would be needed to connect all the evenly distributed smaller demand centers.

As outlook for the potential application of the produced data set, Fig. 6 (b) illustrates how the potential H_2 demands match with the existing natural gas transport network in Germany. Repurposing of individual transport connections from natural gas to hydrogen is an important option to further investigate based on the provided data set of industrial H_2 demands. For example Clees et al. (2021) [7] analyzed the feasibility of the existing natural gas transport infrastructure for hydrogen admixture and transportation of pure hydrogen. Extending this kind of infrastructure modeling with knowledge about site-specific hydrogen demand would greatly improve planning and system analysis.

3.2. Further industrial hydrogen potentials (top-down approach)

The bottom-up hydrogen demand potential of 326 TWh/a calculated above assumes the complete conversion of 615 plants to hydrogen-based processes. This potential covers the major share of the energy-intensive industries. However, there are also potentials for switching to hydrogen in less energy-intensive industries. For these types of potentials, site-

Table 5
Overview of the energetic fuel consumption for the industrial subsectors in TWh/a for 2018 (based on AGEB energy balances [54])

Subsector	Energy carriers per subsector in Germany in TWh/a (2018)		Thereof considered in plant-specific bottom-up analysis in %	Remaining fuel demand for top-down estimate in %	Hydrogen demand (top-down) estimate in TWh/a	Hydrogen demand (bottom-up) estimate in TWh/a	Max. total hydrogen demand in TWh/a
	Gas	Gas + other fuels					
Energy-intensive subsectors							
Basic chemicals	52.03	66.23	–	100	52–66	161	167.5
Metal production (crude steel + metal processing)	47.91	134.59	100	–	–	75	75
Non-ferrous metals	11.61	14.82	25	75	7–10	3.7	14
Glass and ceramics	16.79	17.57	50	50	8–9	8.4	17
Mineral processing	12.97	36.93	33	0–66	0–24	30.7	13
Pulp & paper	19.39	31.01	100	–	–	30.5	31
Refineries	14.31	71.49	–	–	–	17.5	18
Non-energy-intensive subsectors							
Other chemicals	9.49	11.5	–	100	9.5–11.5	–	11.5
Metal subsequent processing	11.24	12.78	–	–	11–13	–	13
Food industry	31.9	36.84	–	100	32–36	–	36
Rubber & plastic goods	6.12	7.06	–	100	6–7	–	7
Machinery	6.65	7.97	–	100	6.5–8	–	8
Vehicle construction	10.8	13.08	–	100	11–13	–	13
Mining & quarrying	1.13	2.28	–	100	1–2	–	2
Others	11.55	28.22	–	100	11.5–28	–	28
Total	249.58	420.88	–	–	156–208	326	482–534

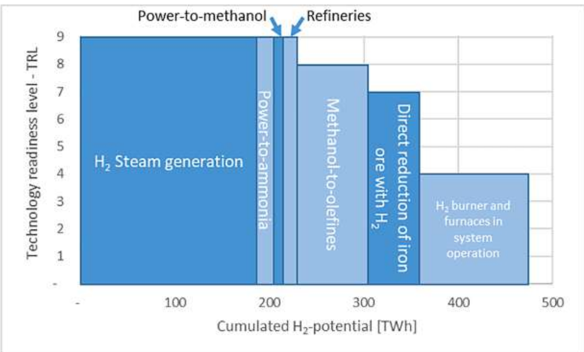

Fig. 7. Hydrogen potentials of the bottom-up and top-down analysis depending on the TRL. Instead of TRL ranges, the lower estimated TRL by technology is shown.

specific information is not available due to the large number of plants and their scattered distribution.

To be able to draw a picture for the whole industry sector, in the following, we estimate the potentials of remaining processes by applying a top-down approach based on publicly available energy balances for 2018, which is shown in Table 5 [54]. Most of the subsectors not included in the site-specific bottom-up estimation use natural gas to cover their energy consumption. However, we consider the substitution of all fuel use including coal, oil and biomass. A brief discussion of the technical potential to switch to hydrogen for remaining energy uses is provided in the following top-down estimation by subsector:

- **Basic chemicals:** For the basic chemicals, the non-energetic gas demand can be completely allocated to the investigated olefins, ammonia, methanol and chlorine. Besides the non-energetic uses, there is an additional demand of about 52 TWh/a for gas and 66.2 TWh/a for fossil fuels that are used energetically to provide process heat - mainly steam.
- **Non-ferrous metals:** For the subsector of non-ferrous metals, only primary aluminum was considered in the bottom-up approach (3.7

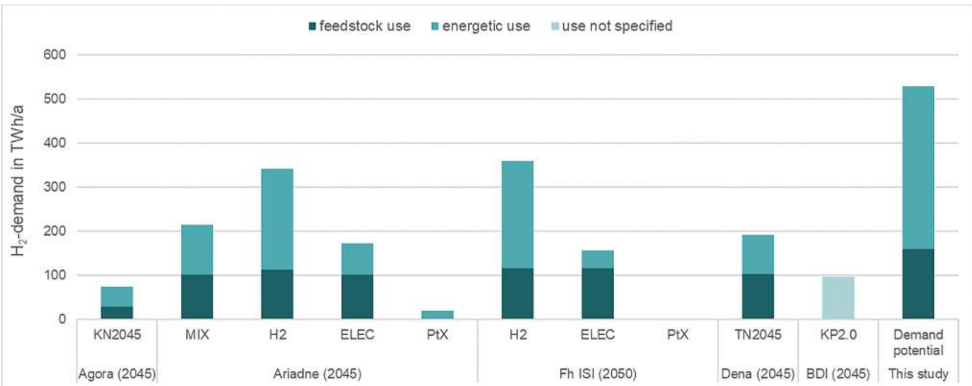

Fig. 8. Comparison of hydrogen demand in relevant scenario studies of climate-neutrality in Germany and potential hydrogen demand from this study.

TWh/a) due to the availability of detailed process-specific and site-specific information. Aluminum processing requires heat and steam during refining, currently primarily generated using fossil fuels. This heat transfer is necessary for the conversion of bauxite into alumina. An alternative for heat production is to use green hydrogen in hydrogen burners and hydrogen-based steam generation technologies.

- **Glass and ceramics:** Apart from glass manufacturing, which is covered in the bottom-up approach, ceramics are the second non-metallic mineral product. Here, high temperature process heat provided by natural gas is assumed to be substituted by hydrogen through burner replacement.
- **Mineral processing:** In the mineral processing industry, about 6 TWh/a are missing compared to the energy balances, due to the fact that only clinker production and lime burning are considered in the bottom-up approach. Here, it is assumed that fossil fuels and renewables can be substituted by hydrogen burner replacements. If it is assumed that only the share of natural gas (33%) is substituted in the mineral processing industry, as this could be done using hydrogen with only minor changes, this would result in in a potential of 12.6 TWh/a.
- **Pulp and paper, metal processing, primary steel:** These subsectors are covered completely in the bottom-up assessment and there is therefore no additional top-down potential. Notably, in primary steel, the potential hydrogen demand is substantially lower (56 TWh/a) than today's fossil fuel demand (134.6 TWh/a). This is mainly because of the more efficient direct reduction process and the electrification of crude steel production via EAF compared to BOF.
- **Refineries:** Altogether, the hydrogen demand in refineries accounts for 22.7 TWh/a in Germany, including 3 methanol production plants that we assigned to basic chemicals in this paper. Without the methanol plants, about 17.5 TWh/a annual hydrogen demand is left. 5 TWh/a of this are produced by SMR. The remaining 12.5 TWh/a are produced internally by refining processes in the reformer and used directly for desulfurization, hydrocracking or hydrotreating. Further, the energetic fossil demand of refineries is not further considered, as there are no reliable forecasts of the future production of refineries.
- **Non-energy-intensive industries:** These were not included in the bottom-up assessment, so a top-down estimation was made based on current energy balances. The largest share is attributed to steam generators, which are widespread in industry, especially in the chemical and food industries [63]. Here, we assume that nearly 100% of the remaining natural gas demand is used for low-temperature process heat for steam generation and could be replaced by hydrogen-based steam generation technologies.

When we combine the results of the bottom-up and top-down estimations, the potential use of hydrogen as a feedstock and as an energy carrier in German industry adds up to between 482 and 534 TWh/a. This includes the results of the bottom-up approach for the energy-intensive industries based on the industrial database of 326 TWh/a with an additional maximum 20 TWh/a for ceramics and other non-ferrous metals (secondary aluminum, copper, and zinc) and an approximation for replacing fossil fuels in the non-energy-intensive industries of between 129.7 TWh/a (substituting only natural gas demand) and 173.2 TWh/a (substituting total fuel demand) depending on the type of substituted fuels. The summarized results of both approaches per subsector are shown in Table 5. The non-energetic use is covered in the bottom-up approach and only applies to the basic chemicals subsector. Here, the bottom-up approach resulted in higher potentials due to the assumed technology switch for olefin production via the MtO process route.

3.3. Technical maturity of hydrogen-based production technologies

The technical maturity of new technologies can be described using the concept of technology readiness levels[2] (TRL, definition of TRLs see Eurostat [75]). In the technology review in **appendix B**, we discuss TRLs for all the technologies considered. Table 2 shows the resulting TRL estimates for all the individual technologies considered. It is clearly shown that technologies with at least TRL 4 are available for all major applications, which ensures that major technical hurdles have already been overcome and that the realization of the hydrogen demand potentials depends mainly on economics and upscaling the available technical solutions.

The considered technologies still show substantial differences in technical maturity ranging from TRL 4 to 9. Thus, while some technologies are still being tested and further developed (H_2 burner technologies integrated in furnace operation), others are already in large-scale operation (H_2-based ammonia synthesis).

Fig. 7 provides an aggregated view of the TRLs of the resulting hydrogen demand potentials. It shows that the major share of the overall hydrogen demand potentials, corresponding to about 360 TWh/a or 75% of the overall potentials, requires technologies with high technical maturity (TRL 7–9). Scaling up such technologies depends mainly on economics and market introduction and not on technical challenges. The main technologies with high TRL are use cases in chemical and petrochemical industries, where grey hydrogen is used at present, but also the use of hydrogen in steam generation and direct reduction for primary crude steel production.

Based on these TRLs, the first short and medium-term implementation for green hydrogen is most likely as a feedstock in the production of basic chemicals and in refineries by substituting conventional steam methane reformers with electrolyzers. If new investments are made into direct reduction plants for primary crude steel production, it is possible to operate them using natural gas as a reducing agent during a transition period until pure hydrogen is economically available in large quantities. The quantity of hydrogen needed for primary steel production in future depends on the development production output, as larger shares of secondary steel production and higher recycling rates can be expected. As the methanol-to-olefins process is very energy-intensive and needs huge amounts of hydrogen, large-scale operation seems more reasonable in a medium to long-term perspective when large quantities of economically produced green hydrogen are available. Deploying the full potential of the methanol-to-olefins route would also require to increase the production capacities of methanol by a factor of about 20 compared to today's production [76]. Technologies for hydrogen-based steam generation are already mature. However, these show possibly key disadvantages in competition with directly electrified steam generators, especially in terms of costs, efficiency and the availability of electricity compared to hydrogen. Large-scale application seems more plausible in the medium to long term due to the availability of green hydrogen as well as the infrastructure required to provide the broadly distributed demand for process heat.

The use of hydrogen burners in furnaces is the main exception in the TRL analysis, with an estimated TRL of 4–5 across the various subsectors and processes. However, despite the low TRL, technical hurdles are not expected to be unmanageable and the low TRL mainly reflects the low availability of hydrogen to establish large-scale demonstration projects as well as less interest in R&D here over the last decades. Using hydrogen as an energy carrier for process heat, except from steam generation, could be done first in glass melting and as a booster fuel in clinker production, as there are also obstacles to using directly electrified technologies in these temperature ranges. Even if the TRL of some of these technologies is currently quite low, as they have not yet been

[2] **Technology readiness levels** (**TRLs**) are used to estimate the maturity of technologies and enable consistent, uniform benchmarking [77].

implemented, their single components already show TRLs of 9. Since the system integration and operation challenges are not considered invincible, development towards market readiness can be expected in the coming years, leading to a rapid increase in TRL. However, intensive R&D programs are required.

4. Discussion

The calculated technical hydrogen demand potentials provide insights into possible spatial distribution of future hydrogen demand as well as the importance of individual sectors and processes. However, we made no forecast about the real or likely deployment and do not consider possible changes in economic structure nor the role of other decarbonization strategies like electrification or stronger circularity. By comparing with recently published prospective scenarios in the following, we put our results into perspective. Fig. 8 shows the resulting hydrogen demand of selected scenarios in the respective year for climate-neutrality from five publications in comparison with our results. For the comparison in Fig. 8 most of the scenarios are expecting hydrogen demand. However, there are of course also scenarios existing in literature without substantial hydrogen demand but going for strong PtX focus, like Ariadne PtX and Fh ISI PtX.

Noticeably, the differences for hydrogen use as feedstock are in a small range, except for Agora KN2045 [77], which assumes electrified steam cracking instead of methanol-to-olefins process route to substitute naphtha-based steam cracking. Comparing energy-related hydrogen demand, the Agora KN2045 is in line with the strong electrification scenarios Ariadne ELEC [78] and Fh ISI ELEC [76], whereas the Dena TN2045 [79] and Ariadne MIX show comparable values for a combined hydrogen and electrification scenario. The strongly hydrogen-focused scenarios Ariadne H2 and Fh ISI H2 show considerable energetic use of hydrogen, but consider changes in production volumes and progress in material efficiency and circularity. Both studies show about 170 TWh/a less hydrogen demands as our hydrogen demand potential. In BDI KP2.0 [80], however, total hydrogen demand of about 100 TWh/a is stated without distinction between energetic use and feedstock use. Besides pure hydrogen, synthetic PtX energy carriers account for an additional demand of 35 TWh/a in Agora KN2045, 65 TWh/a in Dena TN2045 and 173 TWh/a in BDI KP2.0. Overall, the studies present a wide possible range of future hydrogen demand. All scenarios expect a lower demand than the hydrogen demand potentials we calculated. Important reasons for lower demands are changes in production volumes, increasing circular economy with corresponding energy and resource efficiency and deployment of other mitigation technologies.

To assess the realization of the potentials as well as their chronological implementation in industry, criteria like market maturity (TRL), the economic viability of the technologies and the need for corresponding infrastructure require further research.

From today's perspective, it seems likely that green hydrogen and corresponding infrastructure planning may be applied first in processes which already use conventionally produced hydrogen. Here, our results show few sites having considerable potential for demanding green hydrogen. In addition, H_2-DRI for steel production has already been tested at demonstration scale, resulting in a TRL of 7–8 and it is planned to scale this up in several projects. The quantity of hydrogen needed for primary steel production in future depends on the development production output, as larger shares of secondary steel production and higher recycling rates can be expected. However, the German national hydrogen strategy [9] states 55 TWh/a fossil-based hydrogen are currently used in Germany (mainly (petro-)chemical products) and expects to reach 90–100 TWh/a total hydrogen demand by 2030. Especially the aim of ensuring that upcoming investments are spent for climate-neutral technologies like DRI for primary steel production lead to the expectation of increasing hydrogen demand. In the long term, hydrogen is therefore seen for having an important role in securing Germany's position as an industrial player.

The spatial distribution of potential hydrogen demand shows that individual hot spots can be expected and that they will be driven by demand from the steel and chemical industries. This indicates that the planning of supply and transport infrastructure should focus on such hot spots in a first step.

There are higher uncertainties associated with the use of hydrogen in process heat technologies, from a technical perspective but also by considering the huge amount of sites spread widely in Germany. Even if there are no industrial demonstration or large-scale applications in operation so far, there are also obstacles to using directly electrified technologies in high temperature levels. Here, advantages and disadvantages in terms of costs, efficiency and the availability of energy carrier as well as infrastructure and supply aspects required to provide the broadly distributed demand for process heat should be evaluated compared to other technology options.

In summary, the future potential hydrogen demand is largely uncertain. There is huge need for research and detailed investigations of its possible potentials and one such approach was presented in this paper. Further research should take a stronger system perspective by considering also supply of hydrogen as well as the built-up of transport infrastructure and the related costs in an integrated approach. This can particularly help to draw conclusions on the transition period via 2030, when (green) hydrogen supply will still be scarce. Especially more comprehensive scenarios with 2030 perspective with high resolution in spatial distribution of industrial sites with corresponding energy demand and extended analysis to energy system and particularly H_2 transport infrastructure can build on the provided data set.

5. Conclusions

We estimate hydrogen demand potentials using a process-specific and site-specific approach based on the production output of 2018 for the energy-intensive industries in Germany. The literature review shows that technologies using hydrogen for industry decarbonization are under development throughout all industrial subsectors, most of them at least at pilot or demonstration scale. For all the analyzed processes, a hydrogen-based alternative (or retrofit) is expected to become available in the coming decade. We reviewed the literature on the current maturity of hydrogen-based production technologies for the 18 most relevant processes. We included non-energy-intensive industries using a top-down analysis based on the national energy balances for Germany.

In total, we identified a potential hydrogen demand of 482–534 TWh/a for the entire German industry. 326 TWh/a of this result from the site-specific, bottom-up assessment of energy-intensive processes. The top-down estimation using energy balances adds 156–208 TWh/a [54]. If all of these potentials were realized using green hydrogen, around 160 Mt $CO_{2,eq.}$ could be avoided annually (**appendix C**). However, this would entail completely replacing all fossil fuels by hydrogen for process heating and feedstock.

The enormous total potential hydrogen demand of 482–534 TWh/a carries an important message: Huge amounts of renewable electricity will be needed. Producing this amount of green hydrogen via electrolysis would require about 500–600 TWh/a electricity, assuming that electrolyzer efficiency is about 80%. This is more than Germany's total electricity consumption of 500 TWh/a in 2019. On top of that, other sectors will also demand hydrogen. Thus, other decarbonization strategies will need to play an important role. These include the electrification of process heating, but also material and energy efficiency, the transition to a circular economy and carbon capture.

The chemical industry is already using hydrogen as a feedstock for the production of basic chemicals and shows high technological maturity for using green hydrogen on a large scale. In addition, primary steel production via hydrogen-based direct reduction is estimated to have a TRL of at least 7. Together, these two subsectors already show a hydrogen potential of more than 230 TWh/a. Here, only a few sites account for the lion's share of the total site-specific potential. Broken down, 24.5% (80TWh/a) of the site-specific hydrogend demand potentials is allocated at only 3 sites. Together, the 7 sites with the largest potential for hydrogen demand show 150 TWh/a and with 240 TWh/a, the largest 20 sites represent about 74% of the identified potentials and are mostly concerned with the production of basic chemicals and primary steel. On the other hand, the smallest 150 sites only add a potential of 5 TWh/a, equivalent to about 1.5% of the total potential. Thus, a strategy to develop hydrogen infrastructure must involve the largest potential users.

The regional distribution of hydrogen demand shows both a high concentration in a few regions and a relatively broad regional spread. On the one hand, there are 15 regions with a potential higher than 5 TWh/a, reflecting a high density of potentially very hydrogen-intensive industries like basic chemicals and primary steel production. These are partly concentrated in hotspots like North Rhine-Westphalia (around Duisburg), Leuna and Ludwigshafen as well as single sites in a few regions. On the other hand, 141 regions with a low hydrogen potential of up to 1 TWh/a are relatively evenly spread across Germany.

Any plans for the uptake of hydrogen transport and supply infrastructure need to consider this very uneven distribution. A relatively small distribution infrastructure would be sufficient to connect already more than 175 TWh/a of demand with the three major demand centers, while substantially larger infrastructure would be needed to connect all the evenly distributed smaller demand centers.

Our results showed a maximum potential based on the assumption of static industrial production and did not consider other decarbonization strategies like electrification, recycling, CCS or energy efficiency, which will also play a role and certainly reduce the demand for hydrogen. Future studies should look at how the potential hydrogen demand might change in this context. Similarly, we assumed that new hydrogen-based production processes are located at the same sites of today's fossil-based processes. However, there may be more spatial flexibility in the system that should be analyzed in the future.

There is currently still high uncertainty about the future role of hydrogen in the energy system: Expectations are high, but technology diffusion is still in its infancy. Many sectors demand hydrogen, but supply might be limited (at least in the transition period). Thus, further analyses modeling the complete energy system can build on our results by integrating the dataset into energy systems models. In this context, the detailed modeling of hydrogen distribution infrastructure combined with a high resolution of demand and a complete energy system perspective is required to direct policy strategies. Depending on the scarcity and costs of hydrogen production, additional research on prioritization and competition with other decarbonization strategies will be needed to support the transition to a CO_2-neutral industrial production. To sum up, a prerequisite for the successful market diffusion of hydrogen is the creation of suitable framework conditions - both at the political level (regulations and subsidies) and at the company and research level through (further) technology development.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was financially supported by the German Federal Ministry for Economic Affairs and Energy in the context of the project 'VerSEAS', grant number 03EI1018C, and was supported by the Fraunhofer Cluster of Excellence CINES. We want to thank Dr. Matthias Rehfeldt for his helpful feedback and many informative discussions. We are grateful for the financial support.

Appendix A:. Interactive website and open dataset

An interactive website containing a CC BY 4.0 licensed dataset of the site-specific hydrogen potentials has been set up with this paper and is available using the following URL: https://isi.pages.fraunhofer.de/pshp/.

This dataset is going to be extended and updated in future and is available for other research groups for follow-up investigations by using the license and citing this paper.

Appendix B:. Review of the technical maturity of hydrogen-based production technologies

B.1. Burner technologies using hydrogen for process heat

The potentials for the energetic use of hydrogen are related to the generation of process heat, either directly or via steam generation. Several recent studies have been published that investigate the feasibility of burner technologies for firing hydrogen. While some publications report uncertainties about using hydrogen as a fuel due to its combustion properties (high flame velocities and low radiative heat transfer), Lowe et al. (2011) [81] investigated its suitability through heater modeling, burner testing and impact on the fuel system and proved it could be used in process heaters for applications in refineries. Tanneberger et al. (2019) [82] examined combustion efficiency measurements and burner characterization in a hydrogen-oxyfuel combustor with steam dilution, which showed high efficiency. The chemical effect of steam dilution is numerically examined by Lyu et al. (2021) [83]. They found that, depending on the dilution rate and pressure, the chemical effect accounts for about 16.3–20.1% reduction of NO-emissions. Ilbas et al. (2005) [84] modeled combustion of a hydrogen-hydrocarbon mixture and the impact on NOx-emissions. Even if higher NOx-emissions occur due to higher combustion temperatures, this problem can now be solved by recirculating the flue gases to reduce the combustion temperatures or by oxyfuel-combustion with pure oxygen [82,85]. Further theoretical research on mixing natural gas and hydrogen was carried out by Vries et al. (2017) [86] and examined practically by the GWI Essen (2017 & 2019) [85,87]. This confirmed that a mixture of hydrogen in natural gas up to a certain percentage is technically feasible, even if completely replacing natural gas with pure hydrogen is not feasible with the same burner configurations due to different firing characteristics and gas properties (flame velocities, flame length energy density and emissions change). Further, Zhao et al. (2019)

[88] experimentally investigated the influence of the admixture of hydrogen into natural gas on combustion characteristics for burner applications. The highest share in temperature increase can be observed within the first 10% of hydrogen admixture, while fewer CO-emissions are measureable [88]. Dodds et al. (2015) [89] reviewed hydrogen and fuel cell technologies for process heating and stated that replacements of the burner technology and plant redesign are required when firing pure hydrogen due to the combustion properties. The effects of converting natural gas jet flame burners to hydrogen and its influence on heat release rates, jet flame velocities as well as strategies for conversion are modelled and examined in detail by Palacios and Bradley (2021) [90]. Further exploratory research and expert interviews showed that some companies are already using hydrogen burners in their factories or are able to commercially provide burners that are suitable for hydrogen firing [91–93].

For many industrial applications, low-temperature process heat is needed for steam generation, conventionally mainly fired by natural gas. Approaches using hydrogen-based technologies for such applications can be found in the literature. Alabbadi (2012) [94] investigated the direct combustion of pure hydrogen with pure oxygen, which results in high temperature steam that can be cooled down to the required temperature by adding liquid water into the combustion chamber. While there is no scientific literature on further progress in the development of hydrogen-fired steam generators, companies are already commercially offering and selling these solutions [95,96].

In conclusion, based on the literature and the knowledge about the commercial availability of some equipment as well as expert interviews, the TRL was set between 8 and 9 for burner technologies and the use of hydrogen for steam generation. Except for steam generators, applications in furnaces and industrial hydrogen-fired process heaters have not yet been implemented in most of the evaluated industries and are associated with higher uncertainties. These uncertainties mainly refer to very specific process requirements and the unknown consequences of fuel switching for product qualities. The TRL for use in process heat applications has to be set between 4 and 5, following strict definitions for TRL. Despite this, the challenges for system integration and operation are not considered to be invincible in the coming decade, which is why fast development can be expected in the coming years, leading to a rapid increase in TRL.

B.2. Chemical Industry

The basic chemical industry is the biggest user of hydrogen for feedstock applications [97]. In particular, the production processes for basic chemicals (e.g. ammonia, methanol and olefins) show potential for conversion to green hydrogen. In addition, chlorine can also be assigned to the manufacturing of basic chemicals. In the following, we focus on these four products.

Ammonia

About 90% of ammonia, one of the most important inorganic basic materials, is used for the production of fertilizers and has a specific stoichiometric feedstock demand of 0.178 tons of hydrogen per ton of ammonia [12,17].

The production of ammonia consists of two integrated process stages, the synthesis gas process and ammonia synthesis according to the Haber-Bosch process [11,17,98]. The synthesis gas is mostly provided by steam methane reforming of natural gas in Germany [99].

Separating the synthesis gas production from the subsequent Haber-Bosch process makes it possible to avoid fossil fuels (natural gas) by substituting the steam methane reformer with an application producing green hydrogen [15,100-102]. As the Haber-Bosch process and water electrolysis for hydrogen production are at TRL 9, the combination and the complete process concept shows a TRL of 8–9 [101].

Methanol

Methanol is widely used in the chemical industry as an intermediate for a variety of industrial chemicals [103]. In addition, methanol has excellent combustion properties, which allows its use as a fuel or fuel additive in vehicles. The manufacturing of methanol requires a stoichiometric hydrogen demand of 0.189 tons of hydrogen per ton of methanol [11,103].

Conventional production of methanol is based on a synthesis of hydrogen and CO_2 [103]. Therefore, methanol production can basically be divided into three steps: Synthesis gas production, raw methanol production and methanol processing [104]. Most of the industrially produced methanol today comes from the catalytic conversion of synthesis gas [99]. Here, analogous to ammonia, the production of synthesis gas mainly relies on conventional steam reforming [10,11].

For CO_2-neutral methanol production, renewable synthesis gas is needed. Apart from biomass, the availability of which is strictly limited by its renewable potential, large scale applications can be operated by processing green hydrogen with carbon dioxide, e.g. from captured flue gases [105]. Narine et al. (2021) [26] analyzed different process designs for current and future methanol production. Further, Marlin et al. (2018) [27] described and investigated the advantages and disadvantages of direct CO_2 hydrogenation to methanol compared to the conventional production of (fossil-based) syngas. In addition, Castellani et al. (2018) [106] carried out an energy and environmental analysis of flue gas treatment by power-to-gas integration for methane and ammonia synthesis. The process for alternative methanol production shows a TRL of 8–9, as the synthesis as well as the alternative hydrogen production have a TRL 9. However, economic hurdles still need to be overcome [107].

Olefins (Ethylene)

Ethylene and other HVC (high value chemicals), such as propylene and butene, are the starting materials for a large portfolio of other basic materials and products. The following discussion is limited to ethylene as the main product of steam cracking [108].

Ethylene is conventionally produced in the petrochemical industry by the thermal cracking of long-chain hydrocarbons (usually naphtha) in a steam cracker [109]. The composition of the product components can vary depending on the feedstock to be cracked [11,12].

Compared to ammonia and methanol, the renewable production of ethylene using hydrogen is much more complex, since no hydrogen is used in conventional ethylene production [32].

A hydrogen-based alternative production route is the processing of olefins using methanol as an intermediate product (methanol-to-olefins) [32]. First, huge amounts of hydrogen and carbon dioxide have to be converted into methanol, as 2.28 to 2.8 tons of methanol are required per ton of ethylene produced [10,12,13]. In a second step, the methanol is processed to ethylene and other olefins in a synthesis unit. Thus, the specific total energy demand of hydrogen-based ethylene production via methanol-to-olefins (MtO) is higher than the conventional route by a factor of about 5. The TRL of the MtO process is given as TRL 8–9 [11].

Chlorine

Chlorine is produced via chlor-alkali electrolysis. In general, 3 different process types can be distinguished: the mercury process, the diaphragm process, and the membrane process. In Germany, chlorine is mainly produced using the membrane process apart from 2 sites using the diaphragm process. For both the membrane separation and the diaphragm processes, the biggest share of fuel use is needed for steam generation [110].

Here, we assume that 100% of fuel consumption in chlorine production is related to steam boilers, conventionally operated using natural gas, which are potentially replaceable by hydrogen-fired steam generators in future. As hydrogen-based steam generators already show a TRL of 8–9, producing chlorine from hydrogen-fired steam is also estimated to have a TRL of 8–9.

B.3. Refineries

In 2018, 7.6 billion m^3 of hydrogen were used in refineries, which corresponds to 40 % of the hydrogen produced in Germany. Around 78 % of the hydrogen needed in German refineries comes from crude oil refining. This indicates that 22% have to be additionally produced via steam methane reforming [111].

For the processing of crude oil, hydrogen is needed in several process steps. First, hydrotreating for desulfurization of crude oil is based on hydrogen to bond the sulfur in hydrogen sulfide, which can be easily separated. Furthermore, hydrogen is used in hydrocracking to break the carbon–carbon bonds and reduce the length of the molecules to generate more diesel fractions. Some refineries have plants for manufacturing methanol and require additional hydrogen.

Some of the hydrogen demand is met internally from processes (e.g. reformer) that generate it as a by-product [111].

Depending on the development of future production in refineries, the hydrogen required can be replaced by green hydrogen. The amount of hydrogen produced externally in steam methane reformers can be directly replaced by green hydrogen. Should fundamental changes occur in the energy system and feedstock production, the hydrogen demand of refineries could increase strongly for producing synthetic fuels.

We assume refineries take delivery of the liquid, but then possibly “green” raw products (e.g. via pipelines) and further processing to end-products still takes place at todaýs refinery sites. However, hydrogen demand would be much higher if the synthesis of crude products (e.g. naphtha) out of carbon sources (for example CO_2) and hydrogen also takes place in Germany. Our investigation of the hydrogen potential considered both the amount of additional external hydrogen use and the total amount of hydrogen based on today’s production.

B.4. Iron and steel industry

The iron and steel industry is one of the major emitting subsectors in Germany with around 18 Mt of process-specific CO_2-emissions [3]. Steel is one of the most important construction materials and around 30 Mt of crude steel are produced in Germany annually [65]. Two steel production routes can be differentiated.

The primary route uses iron ore and coal to produce crude steel and accounts for about 70% of Germanýs steel production.

In the secondary route, steel scrap is melted in an electric arc furnace, and produces 30% of the steel in Germany. The decarbonization of the primary route is a bigger challenge, while the secondary route is already largely electrified. Thus, we did not include secondary steel production in our analysis of hydrogen potentials.

Blast furnaces are used for the primary production of pig iron. Here, coal is used to produce coke, which is applied as a fuel and a reduction agent [10,33,99]. Subsequently, the molten carbon-rich pig iron is processed into steel in basic oxygen furnaces. Coal and coke account for around 97 TWh/a of the total energy consumption of the iron and steel industry [54].

Replacing fossil fuels in primary steel production by hydrogen in terms of climate neutrality requires investments in completely new plants due to the different processing method involved [10,65]. A number of projects in Germany and Europe have been launched to examine the feasibility of the direct reduction of iron ore with gaseous components - either natural gas or hydrogen. An advantage of direct reduction for decarbonization is that, compared to blast furnaces, about 66% of CO_2-emissions can be avoided using natural gas and that switching the process to renewable hydrogen would be possible when this becomes available on the market [10]. The TRL of direct reduction using natural gas or hydrogen is given as 7–8 [112].

B.5. Non-ferrous metals

The energy demand for the production of non-ferrous metals mostly results from producing aluminum, copper and from foundries. Altogether, they had a natural gas demand of 11.6 TWh/a in 2018 [54], with primary aluminum having the highest energy consumption.

Accordingly, we focused on primary aluminum for the site-specific analysis. This is produced via aluminum electrolysis and shows only limited potential for decarbonization by using hydrogen as most of the process energy demand is already based on electricity. However, the process heat needed within the refining and conversion of bauxite into alumina is conventionally produced using natural gas-fired burners and steam boilers. In general, hydrogen-fired steam generation units show a TRL of 9. There is no information available on whether other hydrogen-based process heat applications are already being tested so these are estimated to have a TRL of 4–5.

B.6. Metal processing

After the production of crude steel, primary shaping through casting is carried out before the metal is formed in a rolling mill. The rolling process is mostly realized in an energy-intensive hot rolling mill at 750–1250 °C and, for some applications, cold rolling of the steel coils is necessary afterwards [47]. Depending on the intended use of the product, further surface treatment (such as pickling, annealing, coating) may be necessary. However, these are negligible from an energetic point of view [35].

In the value chain of metal processing, mainly casting and hot rolling of crude steel show potential for using hydrogen by replacing conventional burners for the generation of process heat with hydrogen burner technologies [34,35]. There are no pilot plants in operation to date, so with the support of experts’ opinions a TRL of 4–5 is assumed for hydrogen burner providing the process heat for metal processing.

B.7. Non-metallic minerals

Glass

Depending on the type of glass, the specific energy demand varies. Even though special glass has the highest energy demand per ton glass produced followed by flat glass, we focus on container and flat glass, as they account for about 85% of the total production volume in the glass industry and could be geographically located on a process-specific level [59].

The production process is almost identical for each type of glass until the shaping process. The melting process, which is mainly fueled by natural gas, consumes up to 85% of the total energy demand of a glass factory and takes place at temperatures between 1,450 °C and 1,650 °C [67,99].

Ireson et al. (2019) [41] investigated alternative fuel switching technologies for glass manufacturing. Hydrogen is considered an option for the decarbonization of the glass industry, although the poor radiative properties of the hydrogen flame is a challenge to further development. Many research groups are developing hydrogen burners for operation with mixtures of hydrogen and natural gas during a possible transition and also for pure hydrogen in the longer term. “P2X” and “HyGlass” are examples of such research projects in Germany [113,114].

If intensive R&D programs are conducted, readiness for 100% hydrogen could be achieved within the next decade, although it may not be economic in this timeline due to high hydrogen production costs [67]. This resulted in our estimated TRL of 4–5 for hydrogen-fired glass furnaces [113].

Mineral Processing

For the manufacturing of cement, clinker has to be produced in rotary kilns with temperatures up to 1450 °C and accounts for 88% of the energy consumed [70]. Most of the required thermal energy is provided by alternative fuels such as the combustion of waste tires, waste oil, animal meal and plastic waste with a 67% share of total fuel consumption [115]. 33 out of 54 cement production sites include the production of clinker, which has the highest fossil fuel demand in cement production. The remaining 19 production sites were not considered in this paper due to their higher share of electricity demand and almost no usage of fossil-based thermal energy [10,70,116]. Cement production sites are often located in the countryside close to limestone deposits [10,70]. The production of lime through burning the hewed limestone is the second most energy-intensive process of the mineral processing industries.

Shares of up to 10% for hydrogen co-firing are not seen as a problem today as this does not change any properties [40]. It seems feasible that the total amount of today’s co-fired natural gas (around 30%) could be replaced with hydrogen. At present, no research is being done in this subsector on using 100% hydrogen, as high shares of secondary fuels (bio-waste) are already used. From a technical point of view, based on section 2.1.2, it seems plausible in future to have rotary kilns for clinker production and shaft furnaces for lime burning fired with synthetic methane or pure hydrogen through burner replacements and a current TRL of 4–5 is assumed.

B.8. Pulp and Paper

For the production of paper, three phases are distinguished: (1) the manufacturing of mechanical and chemical pulp (primary route) as well as recovered fibers (secondary route), (2) the production of paper, and (3) the finishing process [119]. In 2018, the paper industry had an overall natural gas demand of 19.4 TWh/a [54], mainly used for steam generation in the drying and calendering process. Here, paper lanes run through steam-heated cylinders operating at around 140 °C for drying, and are calendered between 80 and 220 °C [117]. The conventional steam generated for the drying and calendering process is assumed to be replaced with hydrogen-based steam generators in this paper.

For paper manufacturing, often only one single SEC-value is given in the literature, ranging between 5.5 and 5.8 GJ/ton [63,67,69]. However, the energy demand for steam generation of the different paper factories varies strongly depending on the type of paper produced [67,99]. For this reason, we tried to be more differentiated and assumed the highlighted values of the ranges given in Table 2, with a TRL of 8–9, as hydrogen-fired steam generators are already commercially available [95,96,118].

Appendix C:. CO_2-avoidance through the realization of hydrogen-based industries

Switching to hydrogen-based processes can make a major contribution towards decarbonized climate-neutral industrial production, if CO_2-neutral hydrogen is used. Considerable CO_2 savings can be achieved by realizing the hydrogen demand potentials identified.

We estimate the resulting potential CO2-avoidance by calculated hydrogen demand potentials. Based on the energy carrier shares per subsector from the energy balances for Germany [54] and the specific emission-factors per energy carrier from UNFCCC [60]. The emissions per sector are calculated as shown in Table 6. A distinction between energy-related and process-related emissions is necessary, as process-related emissions are only avoidable through process changes or the use of alternative feedstocks. We assume that 100% of energy-related emissions are avoided by switching to hydrogen-based process heating. 95% of process-specific emissions can be avoided in primary steel production and around 75% in the production of basic chemicals, which covers a complete reduction of process-related emissions in ammonia production. Altogether, it can be seen that around 160 Mt $CO_{2,eq.}$, which represents 82% of total industrial CO_2 emissions in 2018 (process- & energy-related), are avoidable by realizing all the identified hydrogen demand potentials of between 482 and 534 TWh/a.

Table 6
Process-related and energy-related emissions based on emission factors of the different energy carriers (taken from [61]) and energy carrier shares per sector (taken from [55]) to calculate the possible CO_2-avoidance by realizing the identified hydrogen potentials.

Subsector	Process-related emissions conventional in $MtCO_{2,eq}$/yr.	Process related emissions hydrogen-based in $MtCO_{2,eq}$/a	Energy-related emissions conventional in $MtCO_{2,eq}$/a	Total CO_2-avoidance in $MtCO_{2,eq}$/a
Energy-intensive subsectors				
Basic chemicals	6.73	1.3	17.99	23.42
Metal production	18.06	0.9	42.74	60.80
Non-ferrous metals	1.14	1.1	3.62	3.66
Glass and ceramics	1.83	1.8	3.65	3.68
Mineral processing	18.19	18.2	14.29	14.29
Pulp & paper	–	–	7.63	7.63
Refineries	–	–	20.34	–
Non-energy-intensive subsectors				
Other chemicals	–	–	2.71	2.71
Metal subsequent processing	–	–	2.74	2.74
Food industry	–	–	8.13	8.13
Rubber & plastic goods	–	–	1.52	1.52
Machinery	–	–	1.79	1.79
Vehicle construction	–	–	3.01	3.01
Mining & quarrying	–	–	0.66	0.66
Others	11.23	11.2	6.43	6.4
Total	57.18	34.5	137.27	159.95

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Paper 2

Modelling the transformation of energy-intensive industries based on site-specific investment decisions

published in Nature - Scientific Reports in collaboration with Tobias Fleiter and René Hofmann

A first simple approach presented in Paper II was the basis for establishing a new model to assess industrial transition pathways. This journal paper presents the method of the established open source model with a site-specific approach to investigate the process diffusion in industry transition towards climate neutrality.
The aim of the model is to simulate the interplay of temporal and spatial diffusion dynamics of new processes depending on the cost-competitiveness of competing processes and the availability of infrastructure. Different databases on hydrogen infrastructure topology, industrial sites, and techno-economic parameterisation of industrial processes provide the required model input.
The hydrogen infrastructure contains information on the respective commissioning years. In the current state, plans for a topology development for hydrogen infrastructure according to the plans from the EHB initiative are implemented. The Fraunhofer ISI IndustrialSiteDatabase provides georeferenced industry sites and production capacities that allow site-specific simulation of investment decisions. The techno-economic database contains data on CAPEX, OPEX, energy and feedstock demands, as well as process lifetimes to calculate production costs and estimate process-specific reinvestment cycles. Different settings allow to include simplified policies, such as CO_2 pricing or process bans and to calculate different scenarios by varying the time series for energy price projections. The framework is published open source in line with Paper 2 on GitHub. Data for European primary steel and basic chemical sites are delivered within this open source version as they were published as open data in line with Paper 3.

My contribution: Conceptualisation, Methodology, Validation, Investigation, Formal analysis, Data curation, Software, Writing - Original Draft & Editing, Visualisation.

M. Neuwirth, T. Fleiter & R. Hofmann (2024b). "Modelling the transformation of energy-intensive industries based on site-specific investment decisions". In: Scientific Reports (Sci Rep) *14. ISSN: 2045-2322.*
DOI: 10.1038/s41598-024-78881-7

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Modelling the transformation of energy-intensive industries based on site-specific investment decisions

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The transition towards climate-neutral industry is a challenge, particularly for heavy industries like steel and basic chemicals. Existing models for assessing industrial transformation often lack spatial resolution and fail to capture individual investment decisions. Consequently, the spatial interplay between industry transformation, energy availability, infrastructure availability, and the dynamics of discrete investments is inadequately addressed. Here we present a site-specific approach that considers individual industrial sites to simulate discrete investment decisions. The investment decision is modelled as a discrete choice among alternative technologies with their total cost of ownership as the main decision criterion. Process costs depend on the scenario-specific assumptions, such as energy carrier prices, policy instruments and local infrastructures. The age of production units and their reinvestment cycles are considered the main restrictions on the dynamics of the transition. The results provide high spatial resolution to capture the spatial and temporal dynamics of industry transition under varying process and policy assumptions. The presented model and its results can be coupled with energy system models to assess the implications of site-specific industry transition on energy system related research questions. We conduct an exemplary case study for a transformation pathway of the European primary steel production.

Keywords Modelling, Investment decision, Energy-intensive industry, Innovative technologies, Site-specific, CO_2-neutral industry

Abbreviations

ABM	Agent-based modelling
BF	Blast furnace
BF/BOF	Blast furnace/Basic oxygen furnace
CAPEX	Capital expenditure
CO_2	Carbon dioxide
CCUS	Carbon capture and utilisation or storage
DRI	Direct reduced iron
EHB	European hydrogen backbone
ESM	Energy system model
EU-ETS	European union emission trading system
GHG	Greenhouse gas
GJ	Gigajoule
H_2	Hydrogen
H_2-DRI	Direct reduced iron using hydrogen
IAM	Integrated assessment model
ID	Identifier
ISI	Institute for systems and innovation research
Mt	Megaton
NG	Natural gas
NG-DRI	Direct reduced iron using natural gas

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NUTS	Nomenclature of territorial units for statistics
OPEX	Operational expenditure
SEC	Specific energy consumption
SQL	Structured query language
TWh	Terawatt hours

The industry sector is one of the largest emitting sectors and needs large amounts of fossil energy carriers for energy and feedstock use, especially in heavy industries[1]. Therefore, these industries play a key role in achieving ambitious climate mitigation targets because they are limited by technical restrictions to switch to low-carbon processes. In the future, climate-neutral industries will require large quantities of climate-neutral energy carriers, including electricity, hydrogen, synthetic fuels, and biomass. At the same time, there is still high uncertainty about the technological direction of industry transition and the role of individual energy carriers. Energy system models are used to investigate alternative pathways to inform decision-makers about feasibility and costs. However, as the energy transition progresses, the need for higher resolution becomes increasingly important to accurately capture the complexities and dynamics of industrial transformation and its implications for the energy system.

Thus, understanding of spatial and temporal factors of industry decarbonisation is crucial for developing reliable pathways. The spatial dimension includes the development of the energy demand per energy carrier with georeferenced resolution as well as the consideration and dependence of existing and planned infrastructure.

Temporal factors involve the economic viability of investments and the current industry structure. Economic viability depends on factors like energy carrier prices and investment costs, while current processes, typical reinvestment cycles and the age of individual plants represent the industry structure. Some plants may not have recouped their investment, tying up significant capital and limiting further investments. Additionally, space constraints at many industry sites complicate the construction of new plants. These restrictions on available capital and space make parallel ramp-up efforts challenging. As a consequence, investments into innovative processes are most feasible when the old plant is depreciated and at the end of its life cycle, significantly affecting the temporal ramp-up of new climate-neutral processes.

In general, modelling approaches to investigate energy transition pathways are becoming more detailed to better predict how investments and technological improvements spread in various sectors, such as the electricity market, transport, residential, and industry sectors[2–7].

However, the industry sector is diverse, with various subsectors, products, and processes. Some subsectors require large-scale investments in new production units, while others can achieve fuel switching with smaller investments in individual processes[8,9]. Thus, different modelling approaches exist for representing the heterogeneous industry sector, ranging from assessments of single processes[10,11] to model-based scenarios on subsectors[12–14] or specific products[15–17]. The known instances of industry implementation are often very aggregated due to the integration within complex energy system models (ESMs) and integrated assessment models (IAMs)[18,19]. Examples are the PRIMES model[20] or frameworks such as TIMES[21–23] or MUSE[19], where industries are often reflected by representatives for a stakeholder group. These representatives act based on exogenous assumptions and statistical distributions because the models focus on the mechanisms of entire energy systems rather than on detailed industry sector analysis[24]. Consequently, the respective process diffusion indicates the weighted interests of the representative groups, which does not fit for the entire industry landscape due to its heterogeneity. Most accurate holistic approaches of the entire industry sector so far consider sub-sectoral bottom-up process shares in stock models[25]. Nearly all known industry sector models operate at the national level due to data availability and scope[25,26]. Thus, the spatial distribution cannot be depicted or only estimated retrospectively using different parameters[25]. In summary, existing approaches either set the diffusion of climate-neutral processes exogenously on national level or calculate the diffusion using stock models with strong assumptions on statistical shares[14,25–27]. Consequently, current methods are limited in two aspects. First, without knowledge about the locations the spatial resolution is insufficient to investigate detailed on the linkages between the energy system, the energy infrastructure, and the industry sector. Second, only rough estimates on the diffusion speed can be provided if the current age structure of the individual industrial plants and typical investment cycles are disregarded.

Summarised, research gaps exist in industry sector modelling particularly in addressing the limitations of diffusion of industrial processes and its spatial distribution. To address these challenges in spatial and temporal dynamics, we demonstrate a modelling approach representing individual sites and plants. The model particularly takes into account the georeferenced industrial plant stock of energy-intensive industries and its plant ages in a site-specific bottom-up manner. Our aim is to propose a transparent method based on key parameters such as cost components, energy demand and emissions. Thus, the model code is available as open source in line with this publication and complete industry datasets for primary steel and basic chemicals from Neuwirth et al. [39] are included.

A description about the context and the scope of the model is presented in "Context and scope of the model". "Model overview" introduces the model, its structure and input data. The "Mathematical formulation" presents the main variables and equations that influence the discrete investment decision. For demonstrating a use case of the model, we briefly describe a short case study for the European primary steel sites in "Case study: transformation of European primary steel production according to the structure of the current plant stock". A critical "Discussion" is formulated after presenting the exemplary case study, while "Conclusions and outlook" assesses the possibilities of the model and indicates next steps.

Context and scope of the model

The purpose of this model is to improve the resolution of the industrial sector in the context of energy system analysis. Typically, such sector models are applied in combination with energy system models that cover the broader context of the entire energy system and reflect the market mechanisms for energy markets such as electricity. The models can be applied iteratively by exchanging on energy demand and corresponding prices to imitate the market dynamics. Those market dynamics are covered in ESMs by combining supply effects such as the expansion of renewable capacities, demand sensitivities, and import and export.

Scenario analysis of such individual sector models within the model chains help to provide possible transformation pathways on the demand side, which are mostly aligned with dedicated climate goals. Diffusion pathways for new processes in energy-intensive industries are often set exogenously and nationally according to the given climate goals as data granularity and knowledge about the individual sites within the industry sector is missing.

This modelling approach provides improved spatially highly resolved insights into the structure of the current industries and helps to understand the spatial and timely dynamics for an economic industry transition. In addition to the spatial distribution, the age of the plant stock and the typical investment cycles are the focus of the presented modelling approach when conducting pathways for industrial transformation. Determinants for the investment decision are the availability and existence of energy infrastructure and the economic viability of the considered processes.

The consideration of the mentioned factors are substantiated by the findings of Wesseling et al.[28]. They have examined and characterised the challenges and barriers to the transformation of energy-intensive industries. These industries show high scaling, energy, and capital intensity resulting in long amortisation periods and extended investment cycles, which were identified as critical factors. Prolonged investment cycles offer limited opportunities for technological updates, while low and cyclical profit margins constrain the availability of investment capital. This situation also presents a significant barrier to the successful market entry of new companies, which is a major driver for the diffusion of innovations in other sectors, such as energy and automotive. Additionally, this creates a high dependency on brownfield investments in existing facilities. Besides the restriction from long investment cycles, Wesseling et al.[28] highlight the availability and accessibility of specific resources and energy carriers as significant constraints for the competitive implementation of innovative processes.

The model does not account for additional constraints commonly found in typical diffusion theories, such as network effects, learning effects, and endogenous market mechanisms, which are particularly relevant for consumer goods. Unlike well-documented learning curves for consumer goods, these learning curves are less evident for large-scale industrial plants, and empirical data is notably scarce, especially for the innovative processes targeted by the presented model. The incorporation of endogenous learning effects (reduction in specific costs with increased cumulative production capacity) is also typically not applicable to just a segment of the entire market, as represented in this approach. A significant portion of the learning is global, thus extending beyond the model's scope. Nevertheless, some learning effects can be considered through exogenous assumptions regarding efficiency improvements or the reduction of specific investment costs over time.

In summary, the model serves to address various research questions related to industrial transition in the context of energy system analysis. By coupling with energy system models, these results help improve the understanding of the impacts from the interplay between the industrial sector and other parts of the energy system. The following exemplary research questions, which can utilise the improvements and results from this modelling approach, are raised:

1. How is industrial transformation influenced by the age structure, typical reinvestment cycles, and the spatial distribution of industrial plants?
2. How economically competitive are innovative climate-neutral industrial processes, and how do they change under different conditions, including energy prices and policy instruments?
3. What is the spatial development of industrial energy demand and what dependencies arise concerning infrastructures and import strategies?

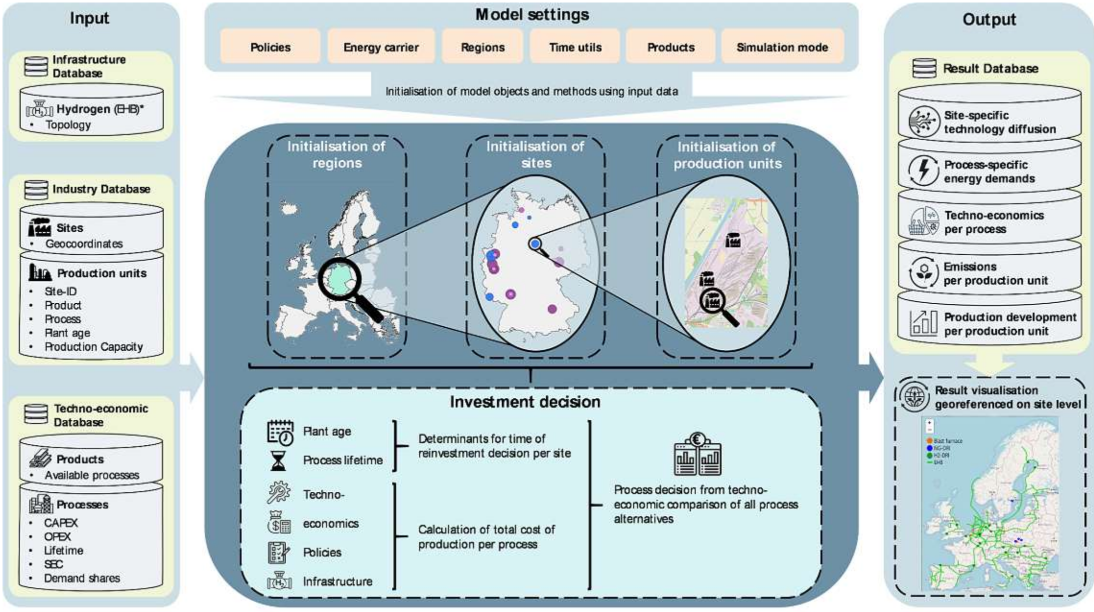
Model overview

According to the previously introduced "Context and scope of the model", the approach aims at a high spatial and process resolution by considering individual industry sites and their production units. Each existing industry site is represented with specific information on geolocation, production units and processes as well as corresponding details such as production capacities and emissions. The chosen simulation approach allows to model the transition of the entire fleet of heavy industry production units of selected countries or regions. The investment decisions depend on the scenario-specific assumptions, such as energy carrier prices, policy instruments and local infrastructures. The decision is modelled as a discrete choice among competing processes with their total cost of ownership as the main decision criterion. The age of production units and their reinvestment cycles are considered the main restrictions on the dynamics of the transition. Figure 1 gives an overview over the entire model, including model input output data.

Software implementation

The model is implemented in Python using commonly known and established packages, listed in the supplementary material. The model classes are defined independently but can be also called by using *mesa*, which is a predefined framework that may act as a scheduler and result visualisation tool in our approach[29].

The model is based on object-oriented programming because it allows the handling of very data-intensive structures in a clear hierarchy with relatively limited operations. In addition, object-oriented programming



* hydrogen infrastructure according to plans from European Hydrogen Backbone initiative

Fig. 1. Model overview including required input data, simplified model procedure, and exemplary outputs.

complies with the requirements of a flexible framework that gives the opportunity to extend towards agent-based behaviour. The most important indicators that distinguish functional programming from object-oriented programming are compared in the supplementary material. Additionally, thorough reviews and discussions on this topic can be found in the literature[30–33]. We applied the factory pattern for decoupling input data and model initialisation as well as the visitor pattern for collecting and storing model results. The factory pattern is a method commonly known and used for object-oriented models[34,35]. It enables the disconnection of the input databases from the model core and allows considerable flexibility in the creation of objects and fast computation, as the model has no need for database connection during the calculations. With regard to the performance of the model and to avoid the occurrence of unused data, only the information needed for the covered regions out of the scenario settings is imported for each model run. Advantages of the established simulation approach compared to an optimisation lie, i.e. in a better representation of individual investment decisions, the faster computing time and no need for external solvers.

Model structure

Figure 2 shows a simplified model overview and workflow of the model procedure. A global main class defines scenario-specific settings, e.g., modelled regions, products, policies, simulation modes, start years, and simulation time steps. Scenario-specific inputs are energy carrier types and price assumptions as well as policy parameters, which manipulate the main drivers of process choice. The model input and settings can be defined externally for each scenario and model run.

During initialisation, these inputs are assigned by the factory classes to the corresponding level in the model hierarchy because they affect different objects. The simulation steps are discrete time steps performed by the scheduler. These methods are flexible and definable but are typically carried out in yearly increments, as that is the most suitable time step for the use case for which the model is built. At each step, the constraints for each region are updated.

In general, the implemented approach classifies its objects and methods into four hierarchical levels. The upper level is the region class, which initiates the regions. The model runs through each region per time step. Within the modelled regions, the industrial sites, undergo a decision algorithm. Each site has one or more production units that manufacture specific products using certain processes. Figure 3 shows an example of a completed template structure for existing industrial sites for the given model hierarchy levels.

Next, we briefly present the necessary data assigned to the corresponding level in the hierarchy:

1. *Region*: This class creates all regions defined in the main class. The definition of a region can be flexible. However, it is reasonable to use internationally predefined levels such as the 'Nomenclature of Territorial Units for Statistics' (NUTS) classification, as this also refers to differences in pricing levels and policy actions. Each region is initialised with a unique identifier (ID). The allocation of the industry sites to the respective region is coupled via this ID. Energy carriers and their associated prices, as time series or parameters, are necessary data inputs for each region. Optional inputs can include any kind of constraint for a region. These may include but

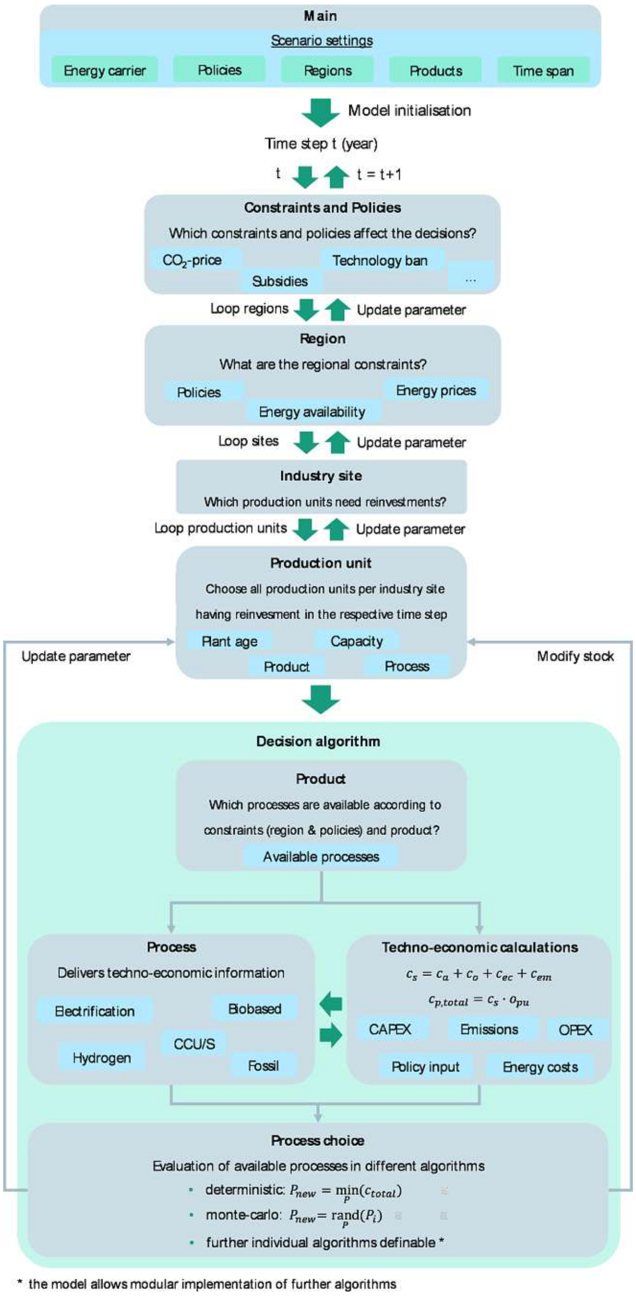


Fig. 2. Simple model overview showing the main elements of the model structure and the functional concept of the process decision per industry site in each time step.

are not limited to different types of policy actions, such as process bans, energy availability, subsidies or taxes. Each region contains a defined list of sites.

2. *Site*: Each site is characterised by a unique ID, the subsector to which it refers, geo-coordinates and production units. The input data for an industry site must include the region ID to allocate region-specific parameters. This enables the individual site to act by using information that is given by the subordinate classes

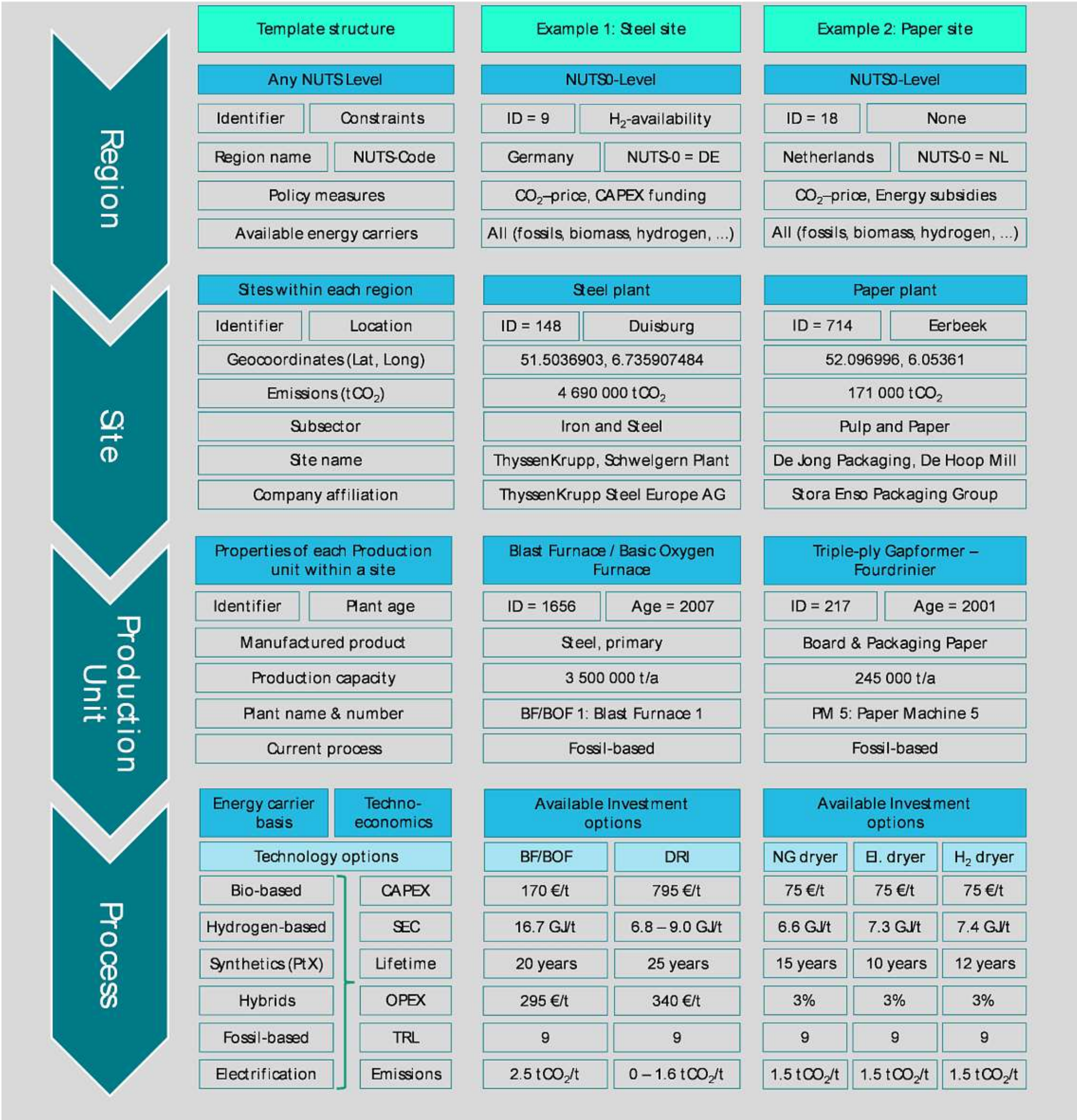


Fig. 3. Filled data input according to the "Model structure" for a primary steel production unit and a board and packaging paper production unit.

for several production units, products and processes. In each time step (usually a year), the model checks whether new investments are required for each site.

3. *Production unit*: Each production unit requires a row of different IDs to connect with. First, site-ID allows mapping to the correct industry site. Knowledge about specific IDs of the manufactured product per production unit enables the connection to the subclass for process-ID options. Further parameters are the yearly production capacity per production unit and the age of the production unit. Based on this, the probability of new investment decisions is calculated, considering the scenario-specific constraints and techno-economic factors at the process level. A production unit can consist of multiple sub-production units, which may produce intermediate products through specific processes. The sub-production units are structured in the same way. One production unit can cover one or multiple industrial plants, depending on the scope of the modelled aggregation. However, given the current data availability, all modelling activities using this model have focused on integrated production plants without sub-production units. Thus, a plant in the following represents a production unit.

4. *Process*: The process class represents the lowest level in the hierarchy of the core model and the initialisation of the industry sites. At the same time, most of the primary data are processed in that part of the model. Here, all specific techno-economic parameters per process identified as alternatives for the production of a specific product are calculated. Most input parameters are needed at the process level. Apart from the product-ID for mapping within the model, time series for CAPEX, OPEX, energy demands, fuel shares and lifetime and emission factors are mandatory.

In the "Mathematical formulation" the rules for the resulting process decision are described. Following this approach, the decision algorithm runs at the site level and is influenced by external constraints (e.g., per region) and site-specific properties. Actions per industry site are carried out if a decision is due whether to reinvest into one of its production units and the corresponding process in the respective year. The basis for site-specific reinvestments is the age of the processes within the respective production units as well as a techno-economic comparison of alternative processes per production unit. The process-specific variables are returned through the hierarchy for processing the techno-economic data in evaluating individual decisions. These site-specific investment decisions based on the age of the individual production units and process-specific techno-economics lead to insights into process diffusion, as the aggregated diffusion dynamics can be explained by individual technology adoption decisions. Variations of the scenario-specific definitions and the exogenous assumptions, such as energy price projections, and the corresponding differences in the results and industrial process decisions give insights into the effects and dependencies. The *mesa* framework supports the applicability of visualisation tools and result creation in combination with the visitor pattern.

Model input data

The model input data are set up as an SQL database and administered by the model via a data interface that connects to the upstream factory classes of each model class. The "Model structure" indicates the need for certain input data, which currently consists of two sources:

First, the Fraunhofer ISI IndustrialSiteDatabase, which includes site-level data for European energy-intensive industries and their main products. The iron and steel, basic chemicals, non-metallic minerals, non-ferrous metals and pulp and paper industry branches are covered with high detail[36–38]. We provide the industry site information for the European primary steel and basic chemical sites, as visualised in Fig. 4a. Definitions of industrial subsectors, products and processes are predetermined by this data structure. The IndustrialSiteDatabase provides data for the individual industry sites with corresponding production units and their products, production capacity, reported EU-ETS emission, plant age and geo-coordinates.

Second, the techno-economic inputs shown in Table 1 are needed for quantifying the different objects in the model structure. In particular, processes need to be described by adding costs such as CAPEX and OPEX, specific energy consumption (SEC) with its type and use and assumptions on future efficiency improvements. For the process-specific techno-economic data, we build on previous work that already address this type of data and extend them with values from recently published literature[25,38]. Scenario-specific inputs are mainly represented by energy carriers with corresponding price assumptions, emission factors and availability per region. Economics for policies such as CO_2 pricing, funding, subsidies or taxes are also defined in the scenario-specific input. The impact of policies, except from process bans, result in price modifications that influence investment decisions through "External cost-influencing factors".

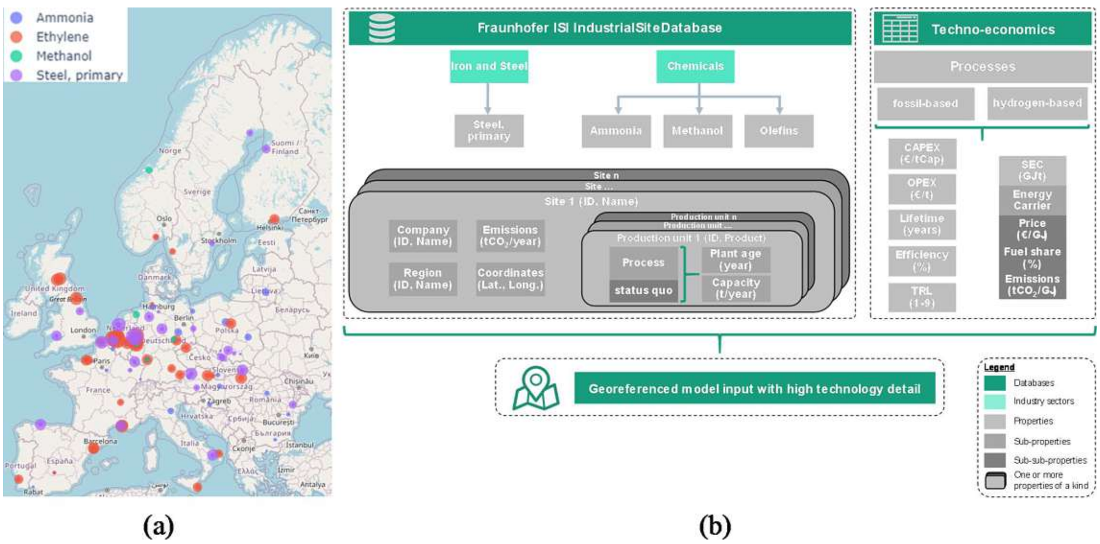


Fig. 4. Matching of the Fraunhofer ISI IndustrialSiteDatabase and techno-economic process data.

Parameter	Description
Process-specific techno-economics	
CAPEX	Capital expenditure (CAPEX) per process in €/t
OPEX	Operational (OPEX) expenditure per process in €/t
SEC	Specific energy consumption (SEC) per energy carrier and type of use in €/GJ
Energetic use	Energy demand for energetic purposes within the process, e.g. direct process heat
Feedstock use	Demand on energy carrier for non-energetic purposes, e.g. fossils in chemical products
Steam generation	Energy demand for steam generation within processes, e.g. drying of paper lanes
Efficiency improvement	Assumed efficiency improvement over time of the respective process in %
Scenario-specific techno-economics	
Energy carrier	Definition of energy carriers used in the modelled industries and processes
Price(-developments)	Price time series per energy carrier in €/GJ
Emission factors	Emission factors per energy carrier in tCO_2/GJ
Availabilities	Energy availability per region in GJ/a
Policies	Policies manipulate investment decisions by setting constraints at different levels
Process bans	Ban for avoiding investments in specific processes per country
CO_2 price	Price(-development) for penalty on emitted CO_2 in €/tCO_2
Subsidies	Subsidies on single energy carriers per country in €/GJ
Taxes	Taxes on single energy carriers per country in €/GJ
Investment funding	Funding on investment for specific processes or projects per country

Table 1. Necessary model inputs used for calculating investment decisions.

These two data sources are automatically matched in a pre-processing step to establish an extensive database dependent on the exogenously defined model settings as input. The data are used to initialise the model according to the template structure of Fig. 3, reflecting the introduced model hierarchy. The required input parameters are connected using the unique identifiers (IDs) of the different levels to initialise the industry sites. Examples 1 and 2 show the detailed granularity of the input data for the respective hierarchy level and model class. The generality of the template structure allows the implementation of very different industries in the same way and simplifies the heterogeneity between them.

A dataset for modelling the entire European primary steel and basic chemical production is published for open source in line with the publication of Neuwirth et al.[39]. We provide these data within the repository of this established approach of the model. Thus, scenarios for the entire European primary steel production and basic chemical industry can be directly applied and modelled.

Figure 4 shows the number of sites and the spatial distribution of the provided data (a) as well as the most important parameters from both sources (b).

Based on the model framework, the whole structure and required input data can be adapted for any other sector or use case. However, the model was established to focus on the industry sector, and the structure of the input templates is well suited for this application.

Model output and visualisation

The aim is to obtain an understanding of the market diffusion of climate-neutral industry processes with a georeferenced site-specific resolution. Accordingly, the model calculates the process-specific energy demands per energy carrier as well as the process- and energy-related emissions per production unit. In addition, the cost components per process, along with the underlying assumptions, are provided as results for analysing the techno-economic indicators. To collect the model results, the so-called visitor pattern is used. Similar to factory patterns, the main advantage is that they work without changing the classes of the objects on which they operate for collecting results to be written. More detailed information on factory and visitor patterns is given in the literature[34,35,40]. For reproducibility, every scenario run is saved in an extra output database. The visualisation of the scenario results is automated by opening a new tab using the python package *mesa-geo*[41], an add-on of the agent-based modelling (ABM) framework *mesa*. This allows us to directly set up dynamic visualisations and simulate the model scenarios on a georeferenced map. In addition, variables and dynamic figures for selected variables reflecting the stage of the simulation can be implemented.

Mathematical formulation

Introduced in "Context and scope of the model", process diffusion in industry faces a variety of sector-specific challenges, such as long investment cycles and high barriers to market entry because of its scale, energy and capital intensity[28]. Moreover, existing economics-based theories and statistical approaches for innovation diffusion have a limited fit to the industry structure, as the restricting parameters differ from those of other sectors. Thus, investment decisions in the energy-intensive industries are more determined by plant age and reinvestment cycles as well as long-term techno-economic driven aspects.

The reinvestment decision is modelled in a discrete manner by simulating the investments of each production unit when it reaches the end of its life in a specific year. As an example, a primary steel manufacturer invests into a relining of its existing blast furnace or into an alternative, such as a direct reduction plant, when the existing blast furnace reaches the end of its lifetime. Regional constraints such as the availability of energy carriers and corresponding prices as well as selected policies affect the decision. Implemented policy options mainly reflect economic aspects and manipulate the decision algorithm through CO_2 pricing, investment funding, subsidies or taxes on energy carriers or by defining process bans. Considering these scenario-specific regional settings, the model calculates the techno-economics for all available processes. Depending on the regional constraints and the respective policies, processes using direct electrification, hydrogen, biomass, carbon capture and utilisation or storage (CCUS) or fossil energy can compete.

The algorithm for the investment decision then chooses the most economic (cheapest) process available for the respective product (Eq. (1)):

$$Inv_p = \min(c_{p,total}) \tag{1}$$

Inv_p process evaluated for new investment for the individual production unit
$c_{p,total}$ total costs per process

The total production cost for each available process (Eq. (2)) recognised for a probable reinvestment within a production unit is derived from a row of cost calculations (Eqs. (3)–(6)), resulting in the specified total cost and the production output per year.

$$c_{p,total} = c_s \cdot o_{pu} \tag{2}$$

$c_{p,total}$ total production cost per process
o_{pu} output/production volume per production unit.

Process-related techno-economics

The basis for the process choice is the total cost of ownership. All calculations are carried out per time step, which is currently implemented as yearly steps. Therefore, the total specific costs per ton of product (Eq. (3)) are calculated as the sum of specific annual capacity costs, specific operational costs and costs for energy carrier use. External influences such as different policy-related aspects or infrastructure access are covered and described in "External cost-influencing factors":

$$c_s = c_a + c_o + c_{ec} + c_{ext} \tag{3}$$

c_s specific total cost per ton of product
c_a specific annuity of investment per ton of product
c_o specific operational costs per ton of product
c_{ec} specific energy carrier costs per ton of product
c_{ext} external influences on specific total cost per ton of product.

Investments per ton of yearly capacity include equipment and supplements needed for the installation of a process and are converted to annual capital costs per ton of product (Eq. (4)) by applying the capital recovery factor and the capacity utilisation factor per year (Eq. (5)).

$$c_a = f_a \cdot c_i \cdot f_{cu} \tag{4}$$

f_a specific capital recovery factor;
c_i specific total investments per ton of installed yearly capacity;
f_{cu} capacity utilisation factor per year.

$$f_a = \frac{((1+r)^i) \cdot r}{((1+r)^i) - 1} \tag{5}$$

i depreciation period

r interest rate

The operational costs consider labour, maintenance and non-energetic resources, e.g., iron ore for primary steel production. Each process is defined by its specific energy consumption (SEC) from the input data and related shares of energy carriers that are used to provide the needed energy. The SEC consists of three dimensions: (i) electricity, (ii) fuel, and (iii) feedstock. Using this information multiplied by the corresponding energy carrier prices for the respective years, the energy carrier costs per ton for each process are calculated (Eq. (6)).

$$c_{ec} = \sum (SEC \cdot sh_{ec} \cdot p_{ec}) \tag{6}$$

SEC specific energy consumption per process
sh_{ec} share of the specific energy consumption per energy carrier
p_{ec} price per energy carrier in the respective year.

External cost-influencing factors

To calculate variations and analyse the effects of external factors such as policies or infrastructure on the process decision and corresponding diffusion behaviour, different implications for economic calculations are realised. More specifically, carbon pricing, subsidies and energy taxes as well as investment funding and infrastructure (currently: European Hydrogen Backbone (EHB) as future hydrogen infrastructure) access can be recognised and applied by a cost factor (Eq. (7)).

$$c_{ext} = c_{em} + c_f + c_{sub} + c_{tax} + c_{inf} \tag{7}$$

c_{em} specific emission-related costs from carbon pricing per ton of product
c_f specific annuity from investment funding per ton of product
c_{sub} specific costs from subsidies on energy carrier per ton of product (< 0)
c_{tax} specific costs from taxes on energy carrier per ton of product
c_{inf} specific annuity from energy infrastructure cost per ton of product

Carbon pricing

The European Union's Emissions Trading System (EU-ETS) is an established instrument intended to reduce greenhouse gas emissions from the participating energy sector and energy-intensive industries[42]. By setting a CO_2 price, companies in the participating sectors are forced to pay for each tonne of carbon dioxide they emit (Eq. (8)).

$$c_{em} = c_{em,ec} + c_{em,p} \tag{8}$$

c_{em} specific emission-related costs per ton of product
$c_{em,ec}$ specific emission costs per energy carrier per unit used per ton of product
$c_{em,p}$ specific emission costs per process.

We represent the ETS as a simple exogenous time series of a CO_2 price that is applied for direct (on-site) emissions from energy carrier use (Eq. (9)) and process-related emissions (Eq. (10)).

$$c_{em,ec} = \sum (sh_{ec} \cdot f_{em,ec} \cdot p_{CO2}) \tag{9}$$

$f_{em,ec}$ specific emission factor per unit of used energy carrier; price per ton of emitted CO_2.
p_{CO2} price per ton of emitted CO_2.

$$c_{em,p} = f_{em,p} \cdot p_{CO2} \tag{10}$$

$f_{em,p}$ specific process emission factor per ton of product.

Indirect emissions from electricity, biomass and district heating are not considered for the CO_2-price, as the model is following the definition of the EU-ETS (only scope 1).

Funding
Funding is a financial support for capital investments. The implementation is realised in two different ways. On the one hand, the funding of individual projects can be directly dedicated to a single industry site (case 1). On the other hand, an amount of money for investment funding per subsector and product for a fixed time period can be set, and a maximum funding rate per production unit is definable (case 2). Reflecting on the mode of operation, the economics of the process choice are affected by a reduction in the CAPEX, as shown in Eq. (11).

$$c_{if} = \begin{cases} \frac{c_{project}}{cap}, & case\ 1 \\ c_i \cdot f_f, & case\ 2 \end{cases} \tag{11}$$

c_{if} specific investment funding per production unit
$c_{project}$ total investments per production unit
cap installed capacity in tons
f_f maximum funding rate per production unit.

The annuity of investment is thereby affected by the specific investment per ton of installed capacity according to Eq. (12).

$$c_f = f_a \cdot c_{if} \cdot f_{cu} \tag{12}$$

Subsidies
Subsidies represent an option as a policy measure for influencing process choice. In particular, subsidies for renewable energy carriers such as hydrogen may support the economy of climate-neutral processes. A reduction in the energy carrier price increases the attractiveness of processes using the subsided energy carrier. The energy carrier price is eased by the provided political subsidy per unit of energy used in the respective process (Eq. (13)).

$$c_{sub} = \sum (SEC_p \cdot sh_{ec} \cdot s_{ec}) \tag{13}$$

s_{ec} subsidy per energy carrier in the respective year.

Taxes
Energy carriers become more expensive by adding taxes on top of the energy carrier price. Therefore, processes needing the respective energy carrier are less attractive due to higher production costs (Eq. (14)).

$$c_{tax} = \sum (SEC_p \cdot sh_{ec} \cdot t_{ec}) \tag{14}$$

t_{ec} tax per energy carrier in the respective year.

Infrastructure
An important aspect for industry when making investment decisions is the availability of energy. Investments in new processes may require alternative energy carriers. Thus, assessing access to the needed amount of the corresponding energy carrier is crucial. To consider these factors and associated costs, existing infrastructures and planned infrastructure projects are fed into the model. As an example for hydrogen, the plans of the EHB initiative serve as an exogenous input to check the possible availability per site by checking the distance to the next pipeline with information about the year of first commissioning for each segment. Based on the calculated distance, a cost factor per distance unit (e.g., kilometre) affects the cost and attractiveness of hydrogen-based processes (Eq. (15)).

$$c_{inf} = d \cdot f_{inf} \tag{15}$$

c_{inf} specific cost per ton of product due to infrastructure costs
d distance between site and next pipeline segment per energy carrier

f_{inf} cost factor per kilometre distance to next pipeline.

Fuel switch

Process choice and investment in processes using new energy carriers entail risks. Thus, flexibility in the use of different energy carriers within restrictive technical limits and hybrid process options is highly attractive. The driver for deciding on the share of used energy carrier per year is the comparison of energy carrier costs seen per industrial site. The total costs are derived from the energy carrier prices, costs for emissions, subsidies and taxes per energy carrier (Eq. (16)).

$$c_{ec,j} = SEC_p \cdot (p_{ec,j} + t_{ec,j} - s_{ec,j} + c_{em,ec,j}) \tag{16}$$

$c_{ec,j}$ specific total cost per energy carrier j per ton of product
$c_{em,ec,j}$ specific emissions cost per energy carrier j.

The share per energy carrier used for the individual fraction of the specific energy consumption can be limited by a minimum and a maximum value per process and can vary between 0 and 1, representing the range from 0 to 100% of covered energy consumption (Eq. (17)).

$$0 \leq sh_{ec,min} \leq sh_{ec,j} \leq sh_{ec,max} \leq 1 \tag{17}$$

$sh_{ec,j}$ actual share per energy carrier
$sh_{ec,min}$ minimum share per energy carrier
$sh_{ec,max}$ maximum share per energy carrier.

In the current state of the model implementation, no heuristic for incremental switching between competing energy carriers is defined. Thus, depending on annual costs, either the minimum or maximum values are chosen (Eq. (18)). If the first energy carrier option is more costly than the second energy carrier option, the processes uses the second energy carrier option to its maximum extend and the first to its minimum.

$$sh_{ec,j} = \begin{cases} sh_{ec,min}, & c_{ec,1} > c_{ec,2} \\ sh_{ec,max}, & c_{ec,1} < c_{ec,2} \end{cases} \tag{18}$$

$c_{ec,1}$ first energy carrier option for the respective process
$c_{ec,2}$ second energy carrier option for the respective process.

Case study: transformation of European primary steel production according to the structure of the current plant stock

We apply and demonstrate the model using a case study for the uptake of hydrogen to supply climate-neutral primary steel production according to the discrete diffusion mechanism based on reinvestments due to the age structure of the current stock. The model results show the possible ramp-up of hydrogen demand in the steel sector and its spatial distribution depending on the EHB. In general, the model results can serve as a basis for a more detailed systemic understanding of process diffusion in industry and its integration into the energy system. The results can help to facilitate the development of policy strategies to support a hydrogen economy in Europe.

Input data and assumptions

We briefly present the current structure of European primary steel production and its key parameters for the conducted case study of the Fraunhofer ISI IndustrialSiteDatabase. Furthermore, the most important scenario input data and corresponding techno-economic assumptions for processes, energy carrier prices and policies are shown and analysed.

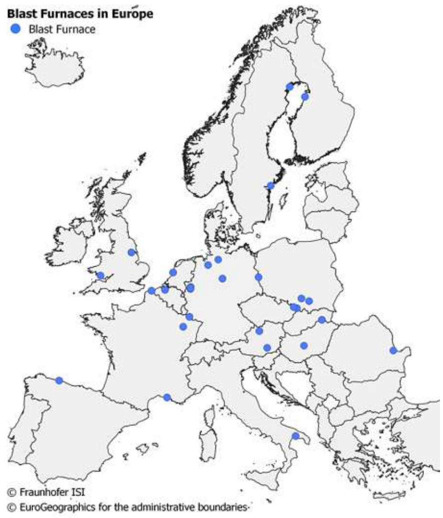
European primary steel sites

Figure 5a lists the structure of primary steel production per country for 2021 from the IndustrialSiteDatabase presented in "Model input data" and its spatial distribution in Fig. 5b.

In summary, currently, 58 blast furnaces are located at 28 sites in the EU27+3, which are dedicated to 15 different countries with a total capacity of approximately 107 Mt of pig iron per year. In total, around 152.1 Mt of greenhouse gas (GHG) emissions are produced per year, and the last refurbishments were conducted from 1971 to 2016.

2021	AT	BE	CZ	DE	ES	FI	FR	HU	IT	NL	PL	RO	SE	SK	UK	Sum
Sites	2	1	2	8	1	1	3	1	1	1	2	1	2	1	3	29
BF´s	5	2	4	14	2	2	8	2	3	2	3	1	3	2	6	58
BOF´s	2	1	1	9	2	1	2	1	2	1	2	1	2	2	3	32
DRI	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1
BF Capacity	5,7	4,5	4,2	32,5	4,5	2,6	12,8	1,3	7,5	6,3	6,1	2,0	4,1	4,9	7,8	106,8
BOF Capacity	7,6	5,0	5,4	37,3	5,4	3,1	11,9	1,7	11,5	7,2	7,6	3,2	3,9	4,4	8,4	123,6
DRI Capacity	0	0	0	0,5	0	0	0	0	0	0	0	0	0	0	0	0,5
Production PI	6,1	4,2	3,9	25,7	4,0	2,5	9,5	0,6	3,9	5,9	3,6	2,1	3,0	4,0	5,8	84,8
Production CS	7,2	4,8	4,6	36,9	4,5	2,6	9,2	0,8	3,9	6,6	4,1	2,3	3,0	3,9	5,9	100,3
Emissions	12,4	7,6	7,7	42,5	5,3	4,2	14,6	1,4	9,6	11,7	5,9	4,8	9,0	4,4	11,0	152,1

(a)



(b)

Fig. 5. Overview of primary steel sites and their characteristics for 2021 in terms of the number of sites, types of plants, production volumes, and emissions (**a**) and the spatial distribution of European blast furnaces (**b**).

Parameter	BF/BOF	DRI/EAF (NG)	DRI/EAF (H_2)
SEC fuel (GJ/t)	16.7	9.0	6.8
SEC electricity (GJ/t)	1.1	2.1	1.7
Lifetime (years)	20	25	25
CAPEX (€/tCap)	170	795	795
OPEX (€/t)	295	340	340
Main energy carrier	Coal	Natural gas	Hydrogen

Table 2. Key process parameters used as input data for producing primary steel via BF/BOF or DRI (according to[45]).

Process and energy assumptions

Current decarbonisation projects and published plans for reducing GHG emissions to reach ambitious climate goals clearly focus on the direct reduction of iron ore[43]. As low carbon investment options in this case study, we allow DRI to be fired by either natural gas or hydrogen, depending on the cost and energy carrier availability.

Table 2 shows the most important parameters and assumptions used for applying the model. Concerning the SEC values, a constant scrap rate of 20% is assumed for all process alternatives[44].

Figure 6a displays the assumed average energy carrier prices per year and corresponding forecasts on the price developments in the countries covered. Without carbon pricing, coal will remain the least expensive, and hydrogen will be the most expensive energy carrier after 2025. The corresponding energy price assumptions for adding recognised carbon pricing are shown in Fig. 6b. Here, the CO_2 price increases linearly from 80€/t in 2022 to 300€/t in 2050. By increasing the CO_2 price, natural gas starts challenging the coal price in the first countries from 2028 onwards, and coal will become the most expensive by 2050. In contrast, hydrogen is already attractive in some countries until 2030, reaches the break-even point compared to coal in 2040 and will be the least expensive starting in 2043.

Case study results

In this case study, we investigate reinvestment behaviour by applying the CO_2 price as a policy (CASE 1) and an additional process ban on the fossil blast furnace process (CASE 2). Specifically, we conduct a short interpretation of the model results by comparing investments and final energy demand between both cases and show the spatial development and visualisation for CASE 2.

Investments

Figure 7 shows the resulting reinvestments by applying the assumption from "Input data and assumptions". For CASE 1 (Fig. 7a), in the early years, blast furnaces remain the most attractive process. In 2028, the first

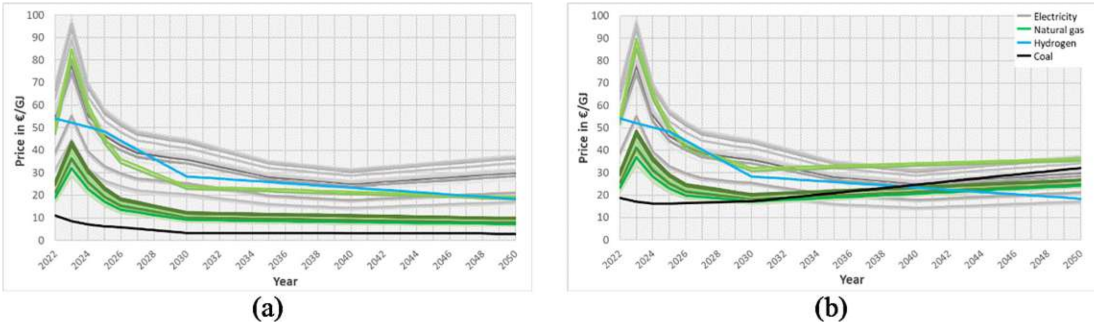


Fig. 6. Assumed price developments for the most interesting energy carriers of the case study: electricity, natural gas, hydrogen and coal without carbon pricing (**a**) and with carbon pricing (**b**).

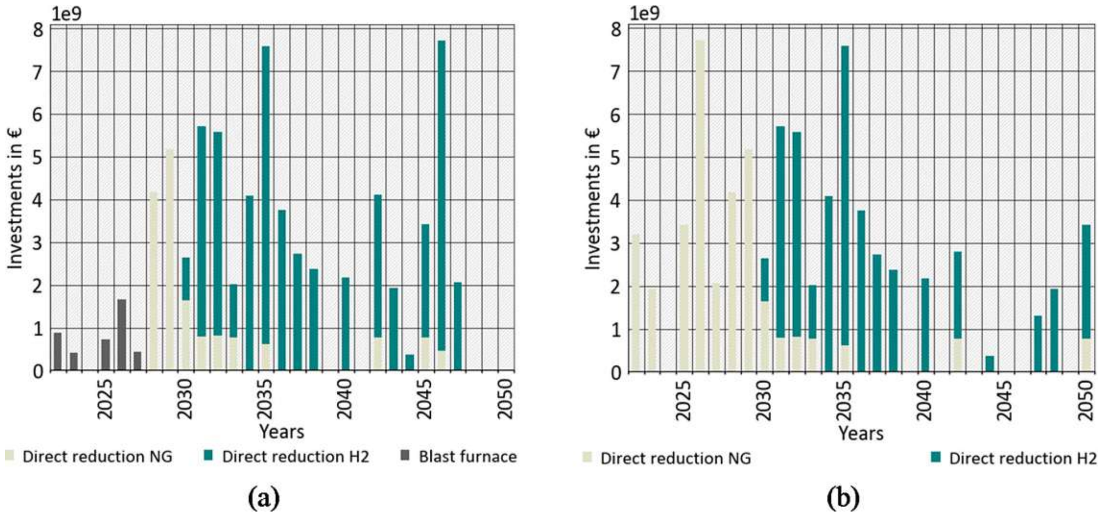


Fig. 7. Investment in primary steel sites according to typical reinvestment without a process ban (**a**) and with forbidden reinvestment in blast furnaces (**b**).

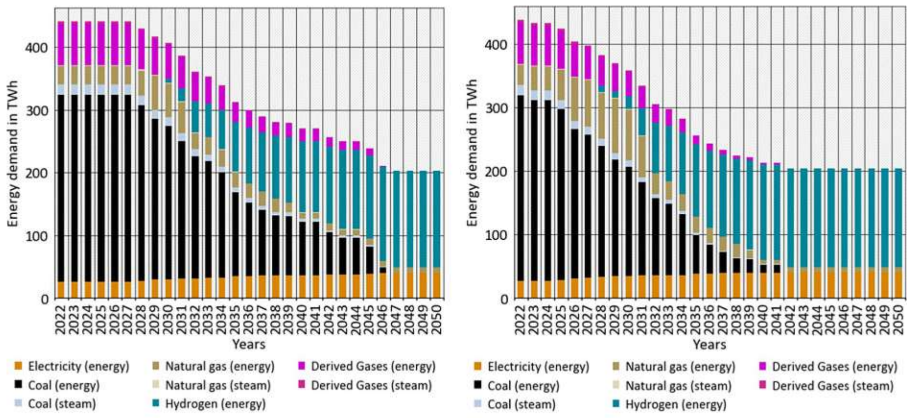
investments into DRI units are made and fired by natural gas. Hydrogen starts to become techno-economically attractive from 2030 onwards. In line with the energy prices in Fig. 6, further DRI investments in the different countries are either planned using natural gas or hydrogen on their first operation. With a theoretical lifetime of 25 years for DRIs, nearly the whole vintage capital stock in Europe will undergo at least one investment decision by 2040. In this case, 17 billion euros will be invested until 2030, of which 9 billion euros will be invested in new blast furnaces. The investment sum until 2040 would result in 52 billion euros of investments. DRI investments from 2045 to 2050 represent the beginning of a second investment phase. In total, 71 billion euros of investments are made by 2050. The cumulative investments are shown in the supplementary material.

CASE 2 (Fig. 7b) realises a process ban for reinvesting in blast furnaces. This reflects the announcements and strategies of European steel manufacturers[43].

Thus, higher investments of approximately 13 billion euros are necessary in the early years until 2030, as DRI investments are more expensive than BF refurbishments. In summary, the calculated investments are 30 billion euros by 2030, 67 billion euros by 2040 and 77 billion euros by 2050.

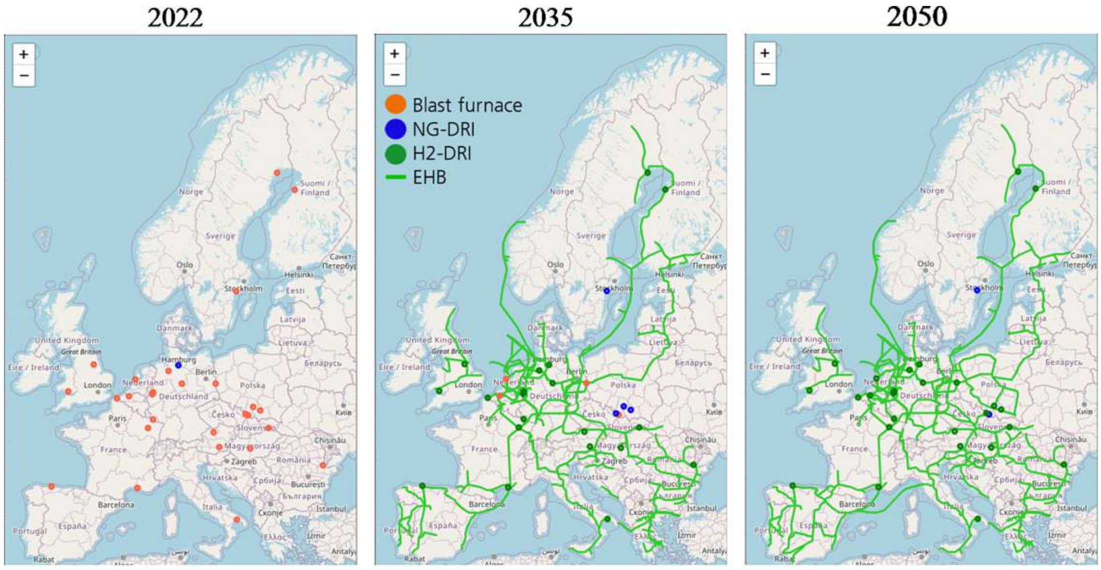
Final energy demand

Early reinvestments into blast furnaces for CASE 1 (Fig. 8a) lead to a high share of coal in the final energy demand until 2030. Between 2028 and 2038, a very linear decrease in coal use can be observed due to substitution with DRI units. During this substitution, natural gas-fired DRI are predominant first, and over time, natural gas will be completely replaced by hydrogen. However, there are no blast furnaces using coal in the system until 2050. In CASE 2 (Fig. 8b), the use of coal will nearly disappear until 2040. A higher natural gas demand results from early



(a) (b)

Fig. 8. Development of the final energy demand for primary steel production in Europe without a process ban (**a**) and with forbidden reinvestments into blast furnaces (**b**).



(a) (b) (c)

Fig. 9. Example of the live visualisation of the model results for a transformation pathway of Europe's primary steel production from the current state (**a**) towards 2035 (**b**) and 2050 (**c**) by recognising the uptake of the EHB.

DRI investments in natural gas. In summary, the difference in the replacement of blast furnaces between both cases results in an earlier phase-out for CASE 2 (Fig. 8b).

Spatial development
In Fig. 9, the visualisation of the transition pathway and process switch of the conducted case study for Europe's primary steel production is shown. Starting from today's capital stock (a), installed blast furnaces are predominant. By 2035 (b), the hydrogen infrastructure plans according to the EHB will be nearly fully established, and individual sites will change processes towards the DRI, either by hydrogen if infrastructure connections are already established or natural gas. At the end of the simulation in 2050 (c), nearly all sites have access to hydrogen according to the plans of the EHB initiative and changed towards H_2-DRI.

More specifically, the diffusion for DRI and its spatial resolution with a fuel switch from natural gas to hydrogen is displayed in Fig. 10. The spatial development for this case study is shown for 2030, 2035 and 2050, but the results are written at a yearly resolution. Until 2030 (Fig. 10a), investments are already being made, especially in Germany, into at least one of the operating production units per site. In central Europe, natural gas dominates the energy use in DRI units. The transitions towards 2035 (Fig. 10b) and 2050 (Fig. 10c) show increasing attractiveness according to the energy price assumptions and further investments in DRI using hydrogen. Only a few sites have no access to hydrogen infrastructure and thus use natural gas in their DRI units until 2050.

Discussion

The presented model enables a site-specific resolution of the current plant stock of the energy-intensive industries. Based on this, scenarios can be conducted and analysed for a detailed examination of the transformation of the European industrial sector. The analysis of investment decisions in new processes and the estimation of future energy demand with the high spatial resolution of the model is valuable for strategic decisions. The model follows a simulation approach as its purpose is to simulate individual investment decisions, which allows to identify existing gaps from investment perspective[39]. Consequently, there is in the current state no optimisation that aims to calculate the optimal investment decisions for the entire system. The sum of investment decisions over the respective period allows conclusions about the spatial and temporal dynamics of the diffusion of industrial processes. The age of the respective plant and the average theoretical lifetime are the basis for individual investment decisions. Although single analyses initially started a similar approach, they did not seem to follow up on this[46].

Nevertheless, the model has some limitations: a need for high quality data and exogenous assumptions, lack of direct interaction between the industry sites, and consideration of market mechanisms.

In general, modelling reliable investment decisions for industrial sites depends on appropriate mechanisms and data gathering. The accuracy and scope of the results depend on the quality of the used data. The Fraunhofer ISI IndustrialSiteDatabase provides detailed input data for energy-intensive industries in Europe, especially for primary steel and basic chemicals sites. The coverage of other energy-intensive industry sectors may lack details such as the age of the plants. Non-energy-intensive industries and cross-cutting processes such as steam generation are not explicitly considered in the data inputs. Depending on the process-specific input data, those cross-cutting technologies can be considered indirectly. The quality of the input data or data gaps can affect the accuracy and meaningfulness of the modelling results.

The level of detail of processes and process chains is adjustable but is subject to a uniform data set and its availability. The comparability of alternative processes for the same product may be affected if the level of detail is inconsistent for competing processes. The model allows to initialise a variable number of sub-production units and corresponding processes for each production unit. Currently, however, industrial plants are modelled as an integrated production unit due to data availability and granularity.

Another limitation is the lack of direct interaction between the industrial sites in the current model state. Although the industrial sites are indirectly connected through central constraints such as policy measures, existing infrastructure, and the availability of energy carriers, direct communication and interaction between industrial plants are currently not implemented. This limitation could impair the model's ability to adequately represent complex dynamic interactions and interdependencies between the industry sites. For example, in the

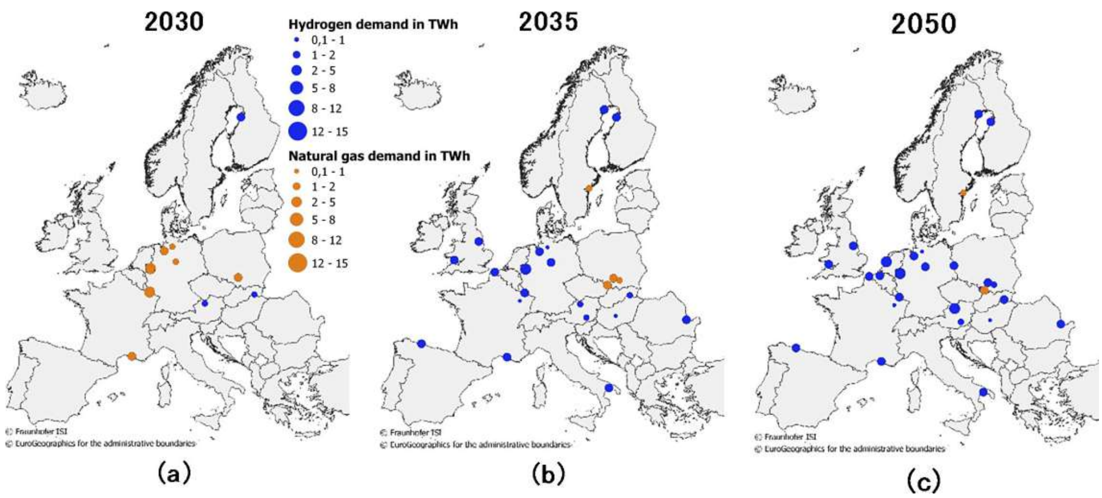


Fig. 10. Spatial development of process diffusion in Europe's primary steel production towards DRI fuelled with natural gas or hydrogen.

steel industry, the decision to build or not build a DRI plant at one site could influence the decision-making at another site.

A crucial and perhaps most significant influence on the results is the techno-economic parameterisation of the processes in combination with the exogenous scenario assumptions on energy carrier prices and policy measures, such as the CO_2 price.

The mentioned limitations affect the model results in several ways. First, incomplete, or inaccurate input data could lead to distorted results, especially if important variables such as the plant age or specific technical details are missing. Secondly, dynamic effects and feedback among the industry sites are limited by the lack of direct interaction between the sites in the current status. The exogenous specification of key influencing factors such as energy carrier prices neglects possible market structures and market mechanisms. However, since the model only represents a part of the market, this limitation is difficult to avoid. Through iterations and feedback of results and parameters with energy system models that also represent other sectors, such market effects can be indirectly included.

Despite these limitations, the model provides valuable insights into specific research questions, particularly those raised in "Context and scope of the model". This model is suitable for analysing scenarios that focus on the investment decisions of individual industrial plants and their temporal and spatial distribution. The site-specific approach supports strategic decisions by estimating when and where industrial actors will need infrastructure for new energy carriers and how energy demand and capacities might develop. Coupled with energy system models, the results obtained can provide a valuable basis for further energy system analyses, such as the need for energy infrastructures, the expansion of energy supply, or the interactions of imports and exports.

Research questions that require a comprehensive view of the entire energy system and participation in market mechanisms can be better covered by integrated energy system models, such as PyPSA[47], TIMES[22,23] or PRIMES[20]. These models offer a system-wide perspective, partially consider global markets, and can better represent the interactions between different sectors and energy carriers. They are also better suited for analysing and recognising long-term and intercontinental or even global developments where the specific details of individual industrial plants are less relevant.

A potential influence on the results could arise from the decisions made during model development regarding the data and methods used. The assumption of predictability of influencing factors such as energy carrier prices partially neglects possible uncertainties regarding future developments, which has an impact on potentially more conservative decisions. In addition, assumptions about economic parameters such as CO_2 prices, investment costs, and energy prices strongly influence the model results and depends on the user. Similarly, specific technical assumptions about the efficiency and availability of new processes lead to distortions if they do not reflect real conditions.

Conclusions and outlook

The site-specific modelling approach offers a framework that is designed to analyse the diffusion of innovative production processes in energy-intensive industries by conducting energy transition scenarios. The aim is to understand the interdependencies between the industry sector and the energy system and their impact on investment decisions of decarbonisation scenarios and to support different stakeholder groups for strategic long-term planning.

The flexibility of the framework allows for a wide range of research questions, with a particular focus on process diffusion and stock turnover, its spatial distribution and infrastructure connection. Detailed knowledge about the current age structure of industry sites enhances the accuracy of the simulations and contributes to a more comprehensive understanding of industry transition dynamics. Different policy designs impact investment decisions and affect the industry's transition to decarbonisation. Georeferenced attributes are used to assess choices based on proximity to energy infrastructure and industry clusters, which may influence process selection. The strength of the model is the modelling of site-specific investment decisions in a detailed spatial and temporal resolution, influenced by multiple factors based on techno-economic aspects.

The open-source interface of the model contributes to the scientific community's understanding of industrial decarbonisation allowing to customise and manipulation of key parameters, facilitating further research, scenario analyses and methodological developments.

In summary, the developed model provides valuable insights into the diffusion of industrial processes at the site level and is well suited for specific strategic analyses. Nevertheless, the context of the system analysis research area and the presented limitations should always be considered when interpreting the model results.

Future developments should focus on enhancing horizontal connections and direct communication between the industry sites to use the advantages of the agent-based framework within the model is implemented. Additional aspects may be the implementation and methodological improvement of further policies, expansion of the data basis, consideration of individual company strategies, and improving the algorithms towards learning effects and for industry site dynamics.

Although the model is established as a simulation approach, implementing individual optimisation problems depending on specific research questions within the simulation workflow offers an opportunity for future directions.

Data availability

All data and source code is available. The model and respective data are available on GitHub referring to this article: https://github.com/fraunhofer-isi/forecast-sites.

Received: 7 May 2024; Accepted: 5 November 2024

Published online: 18 December 2024

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Acknowledgements
This research was carried out as part of the Transience project within the European Union's Horizon Europe research and innovation programme under the grant agreement No. 101137606.

Author contributions
Marius Neuwirth: Conceptualisation, Writing – original draft, Writing – review & editing, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. Tobias Fleiter: Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization. René Hofmann: Supervision, Resources, Conceptualization, Review.All authors have read and agreed to the published version of the manuscript.

Funding
Open Access funding enabled and organized by Projekt DEAL.

Declarations

Competing interests
The authors declare no competing interests.

Additional information
Supplementary Information The online version contains supplementary material available at https://doi.org/10.1038/s41598-024-78881-7.

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Paper 3

Modelling the market diffusion of hydrogen-based primary steel and basic chemical production in Europe - A site-specific approach

published in Energy Conversion and Management with Tobias Fleiter and René Hofmann

This paper assesses possible transformation pathways in dependence of future European hydrogen infrastructure for the entire primary steel and basic chemical production sites in Europe. This publication and the conducted scenarios represent an application of the model from Paper 2.
Validated data for 158 plants at 96 sites for the products considered is used to analyse 16 sensitivities for varying carbon dioxide and hydrogen prices. The respective data is published within the supplementary and included in the repository of FORECAST-Sites. In dependence on hydrogen infrastructure, the transformation is investigated for all primary steel and basic chemical production sites in Europe. The 16 sensitivities differ by varying CO_2 and hydrogen prices. The results show that at least one investment window exists for all plants, while only about one third may have a second investment opportunity before 2050. In addition, more than 30% show reinvestment needs before 2030. Natural gas-based direct reduction of iron ore (NG-DRI) can play a key role and serve as a bridging technology in the transition to the use of green hydrogen for climate-neutral primary steel production. For basic chemicals, especially those where the carbon from fossil feedstocks is embedded within the product, hydrogen prices of 60 €/MWh or below are required for cost-competitiveness of green hydrogen pathways, as carbon prices have only limited effects (scope 1 emissions). The total technical potential for hydrogen use is more than 1000 TWh/yr. Considering current plant ages, reinvestment cycles, infrastructure access, and techno-economic limitations within the sensitivities, hydrogen demand is reduced to 64-507 TWh/yr.

My contribution: Conceptualisation, Methodology, Validation, Software, Formal Analysis, Data Curation, Writing - Original Draft & Editing, Visualisation.

M. Neuwirth, T. Fleiter & R. Hofmann (2024a). "Modelling the market diffusion of hydrogen-based steel and basic chemical production in Europe – A site-specific approach". In: Energy Conversion and Management *322, p. 119117. ISSN: 0196-8904.*
DOI: 10.1016/j.enconman.2024.119117

Energy Conversion and Management 322 (2024) 119117

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Research Paper

Modelling the market diffusion of hydrogen-based steel and basic chemical production in Europe – A site-specific approach

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ARTICLE INFO

Keywords:
Hydrogen
Modelling
Industry
Steel
Chemicals
Technology diffusion

ABSTRACT

Climate-neutral hydrogen is a promising option to replace fossil fuels and reduce greenhouse gas emissions in energy-intensive industries. At the same time, spatial and timely dynamics of hydrogen market diffusion are uncertain. This study simulates the market diffusion of hydrogen-based production routes for the entire European plant stock of primary steel, high-value chemicals, methanol, and ammonia production sites. The model includes a total of 158 plants at 96 sites and explicitly considers hydrogen infrastructure, plant ages, production capacities and reinvestment cycles. Sixteen scenario sensitivities were defined to analyse various future hydrogen and carbon dioxide price pathways. The results show that one investment opportunity remains until 2050 for all plants, while 36% of plants require reinvestment before 2030. The cost-competitiveness of hydrogen-based production varies across products: Methanol and high-value chemicals can only be competitive with hydrogen prices below 60 €/MWh. For steel, a high carbon dioxide price and natural gas-fired direct reduction can mitigate fossil lock-ins using natural gas as bridging option towards full use of hydrogen. The study highlights the risk of reinvesting in fossil technologies without additional policies. The maximum technical hydrogen demand potential is 1000 TWh, but considering techno-economic limitations in the sensitivities, only 64 to 507 TWh can be reached. The planned future hydrogen network matches most reinvestment needs.

1. Introduction

CO_2 mitigation is essential if the European Union (EU) is to achieve its target of being climate-neutral by 2050 and industry currently accounts for 21% of European CO_2 emissions [1]. The EU's ambitious climate targets, embedded in initiatives like the European Green Deal, Fit-for-55 [2] and REPowerEU [3], demand a profound restructuring of its industrial landscape. Central to this transformation is the integration of renewable energy sources and innovative climate-neutral processes. However, one major challenge is the development of a pan-European infrastructure to enable the use of hydrogen, particularly in heavy industries such as steel, high-value chemicals (HVC; containing olefins and aromatics), ammonia, and methanol production. These industries are expected to be major consumers of hydrogen (H_2) in the future [4].

This transformation is not only needed to meet climate targets but is also essential to safeguard the competitiveness of European industries at global level. Energy system modelling tools can be used to support policymakers, researchers, and industry experts in exploring different scenarios and identifying the optimal pathways for this transformation. Assessing the impact of different strategies to guide policy formulation and investment decisions requires a profound understanding of the intricate interplay between industrial strategies and energy system dynamics. Here, the existing modelling tools are limited in terms of the detailed representation of industrial sectors and their transition

Abbreviations: ABM, Agent-based modelling; ASU, Air separation unit; BF, Blast furnace; BOF, Basic oxygen furnace; CAPEX, Capital expenditure; CCfD, Carbon contract for difference; CCS, Carbon capture and storage; CCU, Carbon capture and utilisation; CCU/S, Carbon capture and utilisation or storage; CO_2, Carbon dioxide; DRI, Direct reduced iron; EAF, Electric arc furnace; EHB, European hydrogen backbone; EU, European Union; EU ETS, European Union Emission Trading System; E-PRTR, European Pollutant Release and Transfer Register; GHG, Greenhouse gas; H_2, Hydrogen; H2-DRI, Direct reduced iron using hydrogen; HVC, High Value Chemicals; IPCEI, Important projects of common European interest; ISI, Institute for Systems- and Innovation Research; MtA, Methanol-to-aromatics; MtO, Methanol-to-olefins; MtHVC, Methanol-to-high value chemicals; NG, Natural gas; NG-DRI, Direct reduced iron using natural gas; OPEX, Operational expenditure; SAF, Sustainable aviation fuel; SEC, Specific energy consumption; SMR, Steam methane reforming; TRL, Technology readiness level.

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https://doi.org/10.1016/j.enconman.2024.119117
Received 25 April 2024; Received in revised form 27 September 2024; Accepted 28 September 2024
Available online 16 October 2024

dynamics. Enhancing both the granularity and spatial detail in modelling and data is crucial to better support strategic energy planning.

1.1. Challenges in industry modelling

Each industrial site has unique properties in terms of its history and geography, which have been neglected in recent energy modelling approaches. Industry differs from other demand sectors due to long lifetimes and huge individual investments [5]. However, existing models mostly describe technology diffusion based on statistical changes over time at an aggregated level. Examples are technology stock approaches, in which statistical distribution lead to gradual replacements over time when installations reach the end of their useful lives [6]. Other approaches set exogenous diffusion rates [7]. Varying the parameters and techno-economic assumptions leads to the exploration of different transition pathways, but without taking into account the individual industrial plants or spatial resolution [8]. Even the existing agent-based approaches assume exogenous decommissioning profiles and neglect spatial properties [9]. Only a few approaches in the literature have tried to model the diffusion of new technologies by considering the age structure of the respective plant fleets [10]. Established energy system optimisation models, which represent industrial sectors in an aggregated manner, often provide only sectoral resolution and fail to include site or process details [11]. Industry demands in energy system models are mostly specified on country level [12]. As a result, the existing models are limited about industrial transition at the level of individual plants and sites. In the context of industrial transformation, however, it is crucial to develop a comprehensive understanding of the intricate relationship between spatial and temporal dynamics within the energy system.

A site-specific analysis provides a granular perspective to determine plant-specific energy demand and the energy infrastructure this requires. High spatial resolution is required to better understand the role of infrastructure like hydrogen, gas and electricity networks [13]. Recently, the very first attempts have been made to use site-specific open-source industry data to assess the implications for energy infrastructures [14]. In addition, industry modelling needs to be improved with regard to specific discrete investments and their regional allocation. Modelling discrete reinvestments makes it possible to consider windows of opportunity for investing in climate-neutral processes and the risks of potential fossil fuel lock-ins [5].

1.2. The role of hydrogen in the energy transition

Analysing the potential future role of hydrogen infrastructure in a CO_2-neutral energy system requires industry models with high spatial resolution and a realistic representation of reinvestment cycles. As stated by many recent studies, hydrogen could significantly reduce greenhouse gas emissions and contribute to achieving the EU's ambitious climate goals [15]. The use of hydrogen or its derivatives is prominently discussed in various applications throughout the energy system [16]. Also hydrogen trade flows within Europe and the role of hydrogen storage are relevant in recent research [17]. The EU has taken significant steps towards embracing hydrogen as a key enabler of industrial transformation, driven by the imperatives of decarbonisation, energy security, and economic competitiveness. Hydrogen, especially when produced using renewable energy sources through processes like electrolysis, offers a clean alternative to fossil fuels, and is a viable solution for decarbonising various industrial sectors [18]. Introducing hydrogen as an energy carrier as part of the domestic energy supply requires additional infrastructures and process adjustments in energy-consuming plants [19]. Increasing activities can be observed in political initiatives like REPowerEU [3], numerous publicly and privately funded projects like the Important Projects of Common European Interest (IPCEI) hydrogen programme and initiatives like the European Hydrogen Backbone (EHB) [20]. Many initiatives draw on the existing literature on hydrogen with regard to future demand [18], supply optimisation [21], imports [22], infrastructure needs [23], and global trade [24]. However, these studies are often based on analyses at national or international level and often present hydrogen infrastructures as schematic flows based on a fixed number of nodes [23]. Thus, hydrogen modelling in the demand sectors is often only partly regionalised, e.g. by using distribution keys in a top-down approach [25]. In contrast, detailed regional results exist for the optimisation of renewable power plants and power grids [26].

1.3. Research question and scope

The current literature on energy system analysis indicates a research gap concerning high resolution hydrogen demand from industry at an individual plant site level. Therefore, a novel modelling approach is applied to improve the accuracy of industry representation, which covers the entire fleet of European heavy-industry sites and plants with high spatial resolution. The proposed simulation model provides a flexible method to represent the investment decision-making behaviour of individual industries. The age structure of the current plant stock allows for the recognition of reinvestment cycles in industry, capture limitations of technology diffusion, and provides the necessary level of detail that can be used for further infrastructure modelling and planning. This paper investigates the diffusion patterns of hydrogen-based processes for the industrial production of primary steel, HVC, ammonia and methanol and aims to answer the following research question:

What are the potential diffusion pathways for hydrogen in the production of primary steel and basic chemicals considering restrictions due to the age structure of the current plant stock, policy instruments and infrastructure availability? How do diffusion dynamics compare across different industrial sectors?

The method is based on modelling individual investment decisions as a discrete choice among alternative technologies with total cost of ownership as the main decision criterion. The investigation includes 16 sensitivities for a broad range of hydrogen and CO_2 price trajectories and focus on four selected energy-intensive products. These are steel, HVC, methanol and ammonia, which are all expected to require high quantities of hydrogen for climate-neutral production and a connection to hydrogen transport infrastructure. The focus on the regional scope is EU27 + 3 (Norway, Switzerland and UK) and consider a total of 158 production units at 96 industrial sites. The method can, however, also be applied to other world regions, products and industry sectors. The paper is structured as follows: Section 2 presents the method and main assumptions, and section 3 the results. The analysis of results compares the individual products and the 16 sensitivities in their spatial and temporal dynamics and investigates the underlying driving forces including the role of re-investment cycles and economic competitiveness. Structural differences between the products are shown and risks of fossil lock-ins are identified. After analysing technology diffusion patterns and their spatial distribution, the potential regional limitations of hydrogen availability based on the planned European hydrogen backbone is assed. Based on this, conclusions in terms of investment needs, hydrogen demand and greenhouse gas emissions are summarised. A comprehensive data annex provides a full list of input data and assumptions plus extended data results with high spatial and temporal resolution. These can be used for further energy system analysis.

2. Method and data

This section briefly introduces the method steps for modelling as well as the required data input and its collection as well as relevant assumptions made for this analysis.

2.1. Method

The newly developed model is written in Python and described in detail by Neuwirth et al. [27]. Here, only the core elements required to understand the results in the context of this work are presented. The model considers the specific characteristics of individual industrial sites to simulate investment decisions in new (low-carbon) production processes. Costs are assumptions and depend on the scenario settings, such as energy carrier price projections, policy instruments and local infrastructures. A short description is given in Appendix A. By integrating the choice algorithm into an industry stock approach that tracks individual plant ages and reinvestment cycles are considered the main restrictions on transition dynamics.

To investigate the transition towards hydrogen-based primary steel and basic chemical production in Europe up to 2050, the model uses site-specific information for each plant from the Fraunhofer ISI IndustrialSiteDatabase. This represents energy-intensive industries in detail by merging data from several sources [28]. The focus is on primary steel and the basic chemicals HVC, ammonia and methanol as these industry applications have the highest potential and best technology readiness for using green hydrogen [18]. Figure 1 provides an overview of the methodology used for data gathering and validation as well as of its application and results:

1. **Data gathering and validation:** The database is updated to incorporate the most recent available information for primary steel and basic chemicals sites and validated manually by screening literature, company websites, and press releases as well as information provided by industrial associations and other research projects (section 2.2.1). Conventional and alternative processes are retrieved from previous modelling activities and further literature, see section 2.2.2).
2. **Application of the technology diffusion model:** The validated dataset is used as model input and the theoretical reinvestment cycles of the existing plant stock is analysed. Based on a defined scenario as well as process-specific techno-economic data and dependence on the EHB, the model calculates transformation pathways for 16 combinations of hydrogen and CO_2 prices (4 variations each).
3. **Result analysis:** The results show possible diffusion pathways for hydrogen in primary steel and basic chemicals production. The georeferenced modelling of individual plants with high spatial resolution makes it possible to consider the interplay with the planned hydrogen infrastructure according to the EHB. Parameters like projections of energy demand, investments and emission reduction are analysed.

2.2. Data

The data used as input to the model in this analysis are taken from a database of industrial production sites for the above-mentioned basic chemicals and primary steel merged with site information and process-specific techno-economic parameters. All the data used for this analysis are prepared as supplementary material.

2.2.1. Developing a dataset for the entire fleet of steel and chemical sites in Europe

The Fraunhofer ISI IndustrialSiteDatabase contains information for each plant and site. It is based on matching the European Pollutant Release and Transfer Register (E-PRTR) [29] and European Union Emission Trading System (EU ETS) [30] databases. The spatial scope of the analysis is EU27+3. Additional information for the primary steel production sites was taken from the VDEh steel Plantfacts database [31] for the base year 2015. These data were updated and validated using additional information from Eurofer [32] and Global Steel Plant Tracker [33]. Appendix B **1** shows the detailed number of plants per product and process for each country. 58 blast furnaces (BF), most in combination with basic oxygen furnaces (BOF), are currently in operation at 28 sites across all countries with one plant using direct reduced iron (DRI) fired with natural gas (NG-DRI) in combination with an electric arc furnace

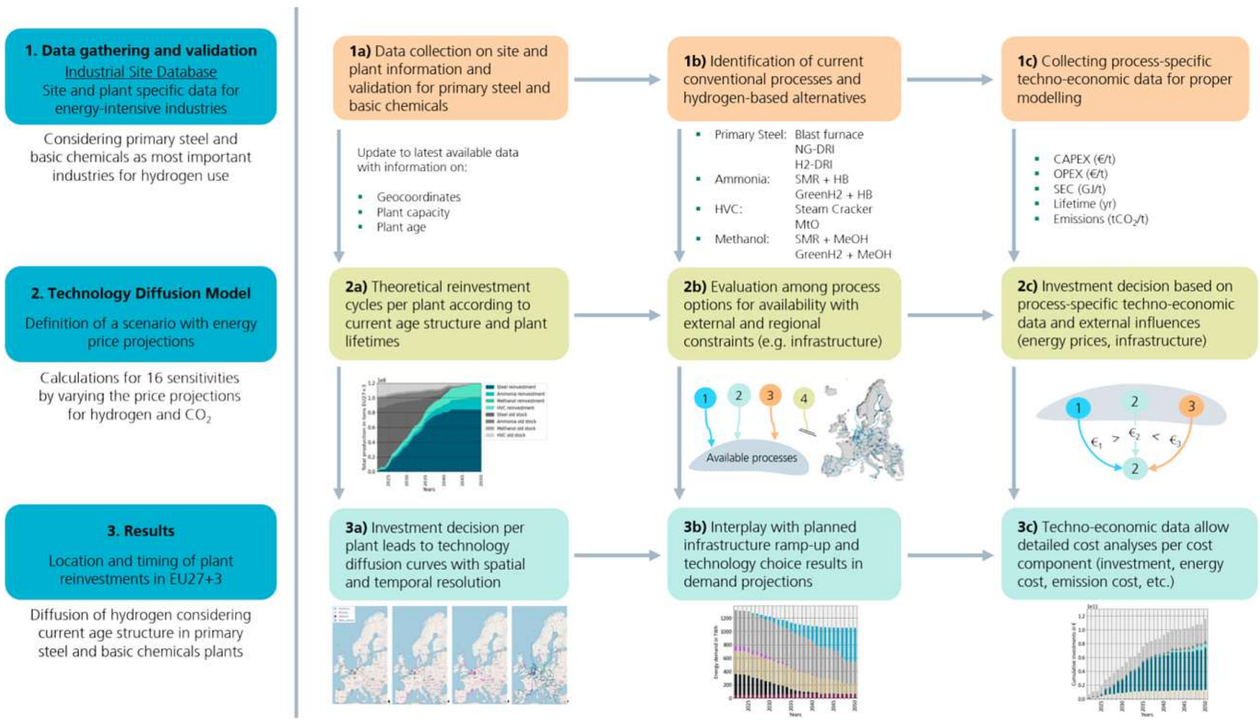

Fig. 1. Methodology for data gathering, model application and results analysis for primary steel and basic chemicals in EU27+3 within this study

(EAF) for primary steel production. Currently, no primary steel plant using hydrogen-based direct reduction (H2-DRI) is in operation. Unlike the iron and steel sector, no known databases exist for the chemical sector. Thus, data collection on parameters like production capacity and age was based on numerous sources per product. For HVC production, cracker capacities are given by Petrochemicals Europe [34]. Further information, e.g. plant age, was gathered from the history sections of individual company websites and press releases (Appendix B **2**). Across Europe, 47 steam crackers operate at 37 different sites. A similar approach was taken for ammonia, where data on capacities and ages were derived from reports [35]. Those were updated and cross-checked with recent publications [36], press releases, and company websites were consulted for manual validation and to incorporate the most recent available information (Appendix B **3**). In total, 45 ammonia plants currently produce at 34 sites. In addition, 7 methanol plants operate at 6 sites, for which information was gathered manually (Appendix B **4**). For both ammonia and methanol, it is assumed that the required synthesis gas is produced via steam reforming (SMR). However, plants for the different chemical products are partly located at the same sites, which leads to a total of 68 sites for the chemical products covered.

In order to be able to carry out a comprehensive and holistic transformation analysis of the selected industrial sectors at a national and a European level, it is first necessary to ensure the completeness of the data with regard to industrial sites and plants. Validation of the completeness based on production capacities is addressed in Appendix C and Appendix D.

2.2.2. *Techno-economic input at process level*

To feed the model with process-specific data in order to run the algorithm on investment decision, literature and process research is conducted to collect data with the necessary granularity.

Here, specification on the chemical compound has to be made. In this study, a typical composition of naphtha-based steam crackers is assumed to be replaced by a combination of methanol-to-olefins (MtO) and methanol-to-aromatics (MtA) process. The average composition is derived from the Prodcom [37] database on European level, showing the following shares for 2019: 41% ethylene, 31% propylene, 5% butene, 15% benzene, 3% toluene, and 5% xylenes. The techno-economic assumptions, such as capital expenditure (CAPEX) or specific energy consumption (SEC), are built by reflecting on these product shares. Following, methanol-to-HVC (MtHVC) describes the combination of both MtO and MtA. Consolidated techno-economic data at process level are listed in Table 1.

As mentioned above, in this analysis, plant age and reinvestment cycles are considered the main drivers of process diffusion in industry. These are evaluated in more detailed in Appendix E. To meet the identified process-specific demands, different energy carriers have specific shares in the individual processes as estimated in Table 2. For the DRI options on primary steel production, shares of natural gas and hydrogen are also partially necessary as reductants.

Based on the assumptions on averaged energy and fuel demand as well as energy carrier shares, the resulting energy and steam demand per plant and site can be used to calculate emissions by applying the emission factor per energy carrier from Table 3.

Electricity and hydrogen do not show emission factors, as their use does not lead to direct CO_2 emissions according to the definition of scope 1 emissions in the EU ETS [30]. Moreover, electricity and hydrogen within this analysis were assumed to be climate-neutral in order to reach the targeted climate neutrality in 2050. The described assumptions and detailed process data make it possible to use the model to conduct simulations of competing processes using the individual industrial sites.

2.2.3. *Scenario assumptions*

Scenarios are defined by setting parameters that are not related to the previously described input data at site and process level. In the presented analysis, national production is assumed to be constant over time. The developed scenario includes a set of prices for fossil fuels and electricity. Hydrogen and CO_2 price paths are expected to have a strong impact on the results of the possible technology diffusion paths for hydrogen-based processes and are also associated with high uncertainty. In total, 16 sensitivities of varying hydrogen and CO_2 prices are applied (4 variations each). These assumptions are briefly described in the following and summarized in Table 4. The scenario represents a realistic "best guess" in terms of fossil fuel and electricity prices. All energy carrier prices have been affected by recent developments. Consequently, the medium to high prices for electricity and fossils decrease strongly until 2030 and then remain on a higher level than pre-crisis from Covid pandemic and the Russian invasion. Hydrogen infrastructure based on EHB plans is considered to provide hydrogen to individual industry sites without capacity restrictions and with maximum availability. The underlying assumption is that an industry site can access hydrogen from the EHB if the distance between pipeline and site is less than 30 km. The

Table 1
Techno-economic model input per process.[1]

Product	Process	CAPEX[2] (€/tCap)	OPEX[3] (€/t)	Lifetime (yr)	Fuel demand (GJ/t)	Steam demand (GJ/t)	Feedstock demand (GJ/t)	Electricity demand (GJ/t)
Steel, primary	BF/BOF	170 [38]	295 [39]	20 [40,41]	16.7 [42]	0.92	0	1.1
	NG-DRI/EAF	795 [38]	340 [39]	25 [43]	9 [4339,44]	0	0	2.1 [4546]
	H2-DRI/EAF	795 [38]	340 [39]	25 [43]	6.8 [45]	0	0	1.7 [45]
HVC[4]	Steam cracker	1700 [47]	60	25 [48]	33.9 [47,49]	0	102.5 [47,49]	1.4
	Methanol-to-HVC	1000 [47]	25	30	0	0.8	138.9 [47,50]	0
Ammonia	Ammonia SMR	550 [51,52]	30	25 [53]	9.4 [54]	-1.8	21.36 [42]	3.2 [55]
	Ammonia H2	110	40	25 [53]	0	-0.9	21.36 [42]	4.8 [47]
Methanol[5]	Methanol SMR	590 [51,56,57]	21 [56]	25 [58]	12.1 [42]	-0.9	22.6 [42]	0.5
	Methanol H2	300 [59]	50	25 [58]	0	0.4	22.6 [42]	0.8 [56]

Primary steel: DRI/EAF greenfield; BF/BOF brownfield.
HVC: MtHVC greenfield; Steam cracker brownfield.
Ammonia: SMR brownfield + HB adjustments; Green hydrogen (grid) air separation unit (ASU) greenfield + HB adjustments.
Methanol: SMR brownfield + methanol synthesis adjustments + purification brownfield adjustments; Green hydrogen (grid) methanol synthesis and purification brownfield adjustments.
[1] Values were derived from thorough literature research and merged with information from experts and own calculations based on the internal FORECAST database.
[2] The values for CAPEX consider greenfield or brownfield investments, depending on the process.
[3] Apart from labour and maintenance costs, operational costs (OPEX) also include material costs that are not represented by energy carriers (e.g. iron ore, scrap and alloying elements for primary steel).
[4] Values on energy and feedstock demand were calibrated to ton of ethylene production for calculations but include the demand for complete HVC production. All energetic values refer to the LHV.
[5] Carbon for methanol production is assumed to be provided at zero cost not specifying the source.

Table 2
Used energy carriers and respective energy carrier shares for fuel and steam and feedstock demand per process.

Product	Process	Coal	Natural gas	Derived gases	Hydrogen	Naphtha
			Fuel and steam shares			
Steel, primary	Blast furnace	0.76	0.07	0.17	0	0
	NG-DRI	0	1	0	0	0
	H2-DRI	0	0	0	1	0
HVC	Steam cracking	0	1	0	0	0
Ammonia	Ammonia SMR	0	1	0	0	0
Methanol	Methanol SMR	0	1	0	0	0
			Feedstock shares			
HVC	Steam cracking	0	0	0	0	1
	Methanol-to-HVC	0	0	0	1	0
Ammonia	Ammonia SMR	0	1	0	0	0
	Ammonia H2	0	0	0	1	0
Methanol	Methanol SMR	0	1	0	0	0
	Methanol H2	0	0	0	1	0

Table 3
Emission factors per energy carrier in tCO_2/GJ.

Energy carrier	tCO_2/GJ
Electricity	0
Coal	0.096
Natural gas	0.056
Derived gases	0
Naphtha	0.076
Hydrogen	0

EHB is assumed to provide sufficient long- and short-term storage capacity (e.g., via underground cavern storage), and the hydrogen prices include this. In the long term, this is regarded as the cost-optimal solution compared to decentralized storage solutions. In the short term and during the construction of the hydrogen grid, decentralized generation and storage solutions at the industrial site might play a certain role, which is not considered in this analysis.

The qualitatively described key assumptions from Table 4 are visualised as a time series for detailed comparison. As an in-depth analysis of all countries within this publication is too extensive, the focus is set on Germany in parts of the results section. Germany is the country with the highest number of sites and plants for the considered products.

Therefore, the price assumptions for Germany are highlighted within the shaded price range for all countries for electricity, natural gas, naphtha and coal (Figure 2) as well as CO_2 and hydrogen (Figure 3). All sensitivities for hydrogen prices assume a decreasing trend until 2050. There are variations for the CO_2 price, which increases from roughly 80

Table 4
Scenario definitions and corresponding key assumptions

Indicator	Unit	Quantitative example: Germany			
		2022	2030	2040	2050
Description	*Medium short-term price shocks due to Covid pandemic and Russian invasion of Ukraine without huge long-term effects. This scenario reflects a realistic or best guess estimation concerning conventional energy prices*				
Electricity price	€/GJ	62.7	41	37.6	34.2
Natural gas price	$€/GJ_{LHV}$	18	8.7	7.8	7
Naphtha price	$€/GJ_{LHV}$	22.6	13	12.7	12.4
Coal price	$€/GJ_{LHV}$	4.5	3.4	3.2	2.9
Fuel oil price	$€/GJ_{LHV}$	22.6	13	12.7	12.4
Energy availability	GJ_{LHV}	unrestricted	unrestricted	unrestricted	unrestricted
Production	ton	2019 calibration	2019 calibration	2019 calibration	2019 calibration
Sensitivities	*Sensitivities are conducted with same assumptions on electricity and fossil energy prices. They differ in hydrogen and CO_2 price assumptions (4 variations each) and thus result in 16 sensitivity combinations.*				
Variation		v1 / v2 / v3 / v4	v1 / v2 / v3 / v4	v1 / v2 / v3 / v4	v1 / v2 / v3 / v4
Hydrogen price	$€/GJ_{LHV}$	27 / 37 / 45 / 57	20 / 27 / 33 / 40	17.5 / 23.5 / 29 / 35	15 / 20 / 25 / 30
CO_2 price	€/GJ	80 / 80 / 80 / 80	129 / 143 / 157 / 171	189 / 221 / 254 / 286	250 / 300 / 350 / 400

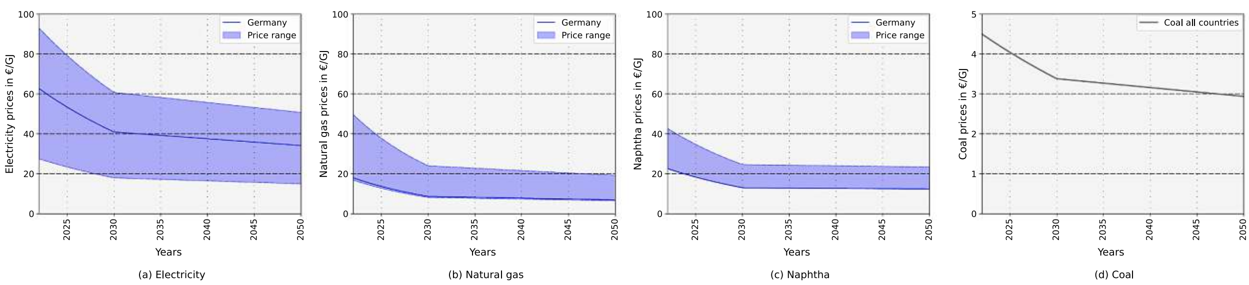

Fig. 2. Electricity and fossil price ranges for all countries considered. The price series for Germany is highlighted as an example of trajectory of one country.

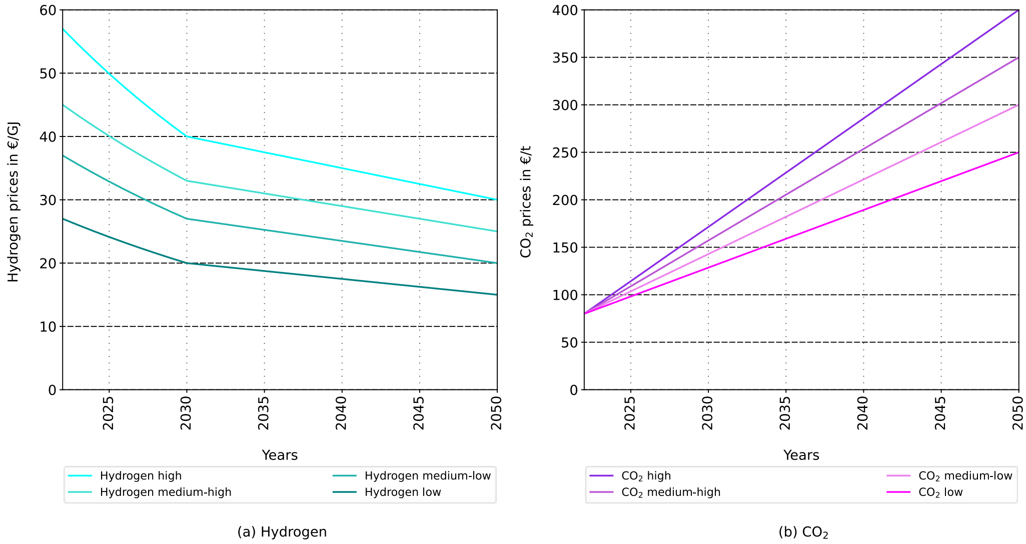

Fig. 3. Sensitivities on hydrogen and CO_2 prices for all countries

€/tCO_2 at present to different higher prices by 2050 (250 €/tCO_2, 300 €/tCO_2, 350 €/tCO_2, 400 €/tCO_2).

The variations shown in Figure 3 for the hydrogen price seem to be very optimistic, especially the lower price paths. However, recent studies indicate that hydrogen prices could fall to between 15 and 20 €/GJ , which is the range of the two lower hydrogen price paths for 2050 in this analysis [60].

Other studies show wider ranges, but also the prospect of future hydrogen production costs in Europe below the assumptions made here [61]. Even lower hydrogen production costs are published in latest literature including salt cavern storage [62], but additional costs for transport and without stating the amount of hydrogen that can be produced to those low-cost conditions.

3. Results

This section presents and analyses the results of the scenarios defined in section 2.2.3 on an aggregated European level. However, as the model calculates all the results bottom-up at plant level for each individual site and plant, more detailed results per country are provided in table and bar chart format in supplementary excel files.

3.1. Market diffusion drivers

Reinvestment cycles based on the plant ages of the existing plant stock and economic competitiveness are analysed concerning their impact on the market diffusion.

3.1.1. Reinvestment cycles

The model only allows new investments in hydrogen-based processes if the existing process reaches its assumed end of life. Consequently, the theoretically cumulated phase-out of the current plant stock determines the maximum diffusion speed for new investments (not considering early replacement or retrofitting). Figure 4 shows the theoretical reinvestments for all plants in EU27+3 for the considered products. It becomes clear that, in theory, complete replacement of the entire plant fleet is still possible by 2050 by following theoretical reinvestment cycles. However, at the same time, it is clear for most plants that there is not more than one reinvestment cycle remaining until 2050.

Across all plants, about 39% of production capacity requires replacement until 2030 and about 68% by 2035. This early need for reinvestments constitutes a high risk of lock-ins in fossil fuel-based processes, because hydrogen-based processes are not yet economically competitive (section 3.1.2). In addition, hydrogen may not be available in sufficient quantities.

Comparing the individual products reveals a diverse picture (Figure 4). Around 42% of blast furnaces, 41% of steam crackers (HVC production), and 51% of methanol plants require reinvestments by 2030. In contrast, only 22% of European ammonia plants need reinvestments by 2030.

Theoretically, a lifetime of 20 years as assumed for blast furnaces would allow for a second cycle of reinvestment before 2050 for some

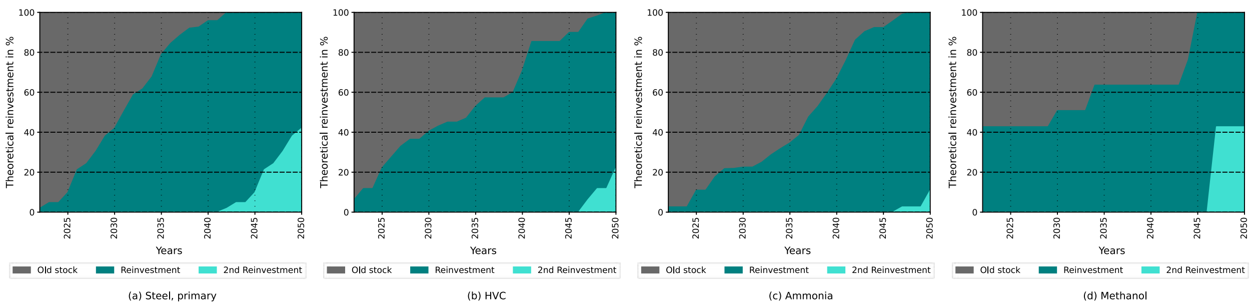

Fig. 4. Theoretical phase-out of current conventional plant stock in EU27+3 according to plant age and typical lifetimes for primary steel, HVC, ammonia and methanol plants

plants. For the other products, lifetimes are expected to be 25 years (Appendix E), which reduces the potential for a second reinvestment cycle. Thus, the potential to replace early reinvestments in fossil-based processes before 2050 is very limited.

To better understand the risk of lock-ins, the following sections assess the economic competitiveness and the availability of hydrogen infrastructure over the entire period.

3.1.2. Economic competitiveness

The economic competitiveness of hydrogen-based processes varies across the countries depending on their national energy prices. This variation is an important factor that explains the differing speed of technology diffusion in Europe. This assessment focuses on Germany, which has the highest manufacturing capacity for the investigated products with 39 plants at 25 sites (Appendix B **1**). CO_2 avoidance costs are investigated as the main indicator for the economic competitiveness.

Figure 5 compares the CO_2 avoidance costs for the three steelmaking processes. The break-even points for switching from BF to NG-DRI are around 120 to 130 €/tCO_2, which is before 2030 for all the assumed CO_2 price trajectories. The break-even point for switching from BF to H2-DRI ranges from 100 to 180 €/tCO_2 and is highly dependent on the hydrogen price. For both options, the high CO_2 intensity of coal-fired BF supports the early competitiveness of DRI. Switching from NG-DRI to H2-DRI is even more dependent on the hydrogen price, as the CO_2 price has a lower impact resulting from a reduced CO_2 intensity of NG-DRI of about 68% compared to BF. High hydrogen prices increase avoidance costs to 180 to 260 €/tCO_2, delaying the break-even point to after 2035. However, hydrogen becomes attractive in all sensitivities before 2050, even with high hydrogen prices (Figure 5 (c)). The early competitiveness of NG-DRI helps the steel industry to avoid lock-ins, serving as an interim solution towards climate neutrality. Once hydrogen is competitive and available in sufficient quantities, it can replace natural gas without significant additional investments.

Similarly to the NG-DRI to H2-DRI transition, for ammonia production, the hydrogen prices significantly impact the break-even point (Figure 6 (a)). In both cases, the cost difference between natural gas and hydrogen is the main determinant. A different situation is observed for HVC and methanol production. Converting methanol production to the direct use of green hydrogen is only competitive with low hydrogen prices and high CO_2 prices, resulting in a late break-even point, which is even after 2050 in some sensitivities (Figure 6 (b)). This effect is even more pronounced for the conversion of HVC (Figure 6 (c)), where the switch from naphtha-based steam crackers to MtHVC using climate-neutral methanol becomes cost-competitive only after 2043 at the lowest hydrogen prices. In both cases (methanol and HVC) a large share of the fossil carbon is bound as a raw material and embedded in the product rather than emitted during production, which limits the impact of the CO_2 price. Under current EU Emissions Trading rules, the respective chemical companies do not need CO_2 allowances for the carbon embedded in their products [30]. The resulting emissions occur at a later point in the value chain, such as during waste incineration.

To conclude, the combination of the high impact of the CO_2 price on coal-fired blast furnaces and the availability of a transitional process with NG-DRI helps to mitigate the risk of fossil lock-ins in the primary steel production. In contrast, the analysis of cost competitiveness shows that especially hydrogen-based alternatives for methanol and HVC will not be cost competitive in the medium term and require both a high CO_2 price and a low hydrogen price. It is very likely that hydrogen-based alternatives will not yet be competitive when reinvestments are required in the coming decade, and the pressure to reinvest in fossil fuel-based processes will be very high. Avoiding fossil lock-ins here will require additional policy measures.

3.2. Market diffusion results

The temporal dynamics as well as the spatial resolution and the impact of the planned hydrogen infrastructure on the plant-specific market diffusion of hydrogen-based processes are analysed.

3.2.1. Temporal dynamics

The results for the technical reinvestment cycles (section 3.1.1) and the competitiveness of hydrogen-based processes (section 3.1.2) determine the technology diffusion across the 16 sensitivities defined. The sensitivities vary in terms of the price for hydrogen and CO_2, which affects the economic viability of the various reinvestment options. Figure 7 shows the technology diffusion over time for all price combinations and aggregated for the four products considered. The vertical axis of rising CO_2 price leads to earlier diffusion and higher shares of hydrogen-based processes, while falling prices for climate-neutral hydrogen on the horizontal axis have an even stronger impact. However, this effect may change with different hydrogen and CO_2 price paths. Low CO_2 and high hydrogen prices result in late and low diffusion of hydrogen-based processes from around 2040 onwards, with NG-DRI taking early large production shares due to lower emissions compared

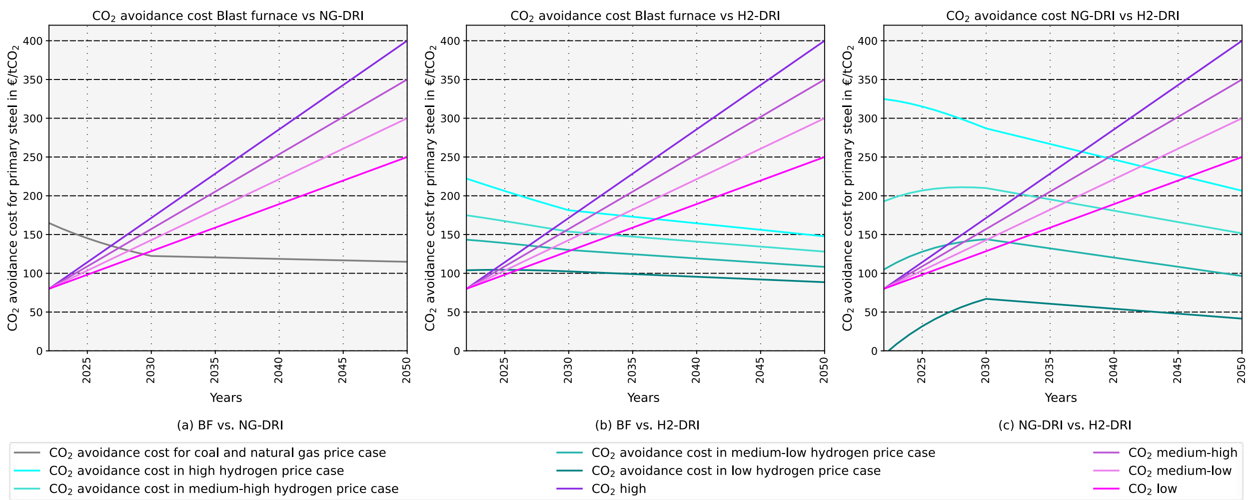

Fig. 5. CO_2 avoidance costs for primary steel (BF vs. NG-DRI (a), BF vs. H2-DRI (b), and NG-DRI vs. H2-DRI (c)) production in the four different hydrogen price sensitivities and comparison to the four defined CO_2 price paths

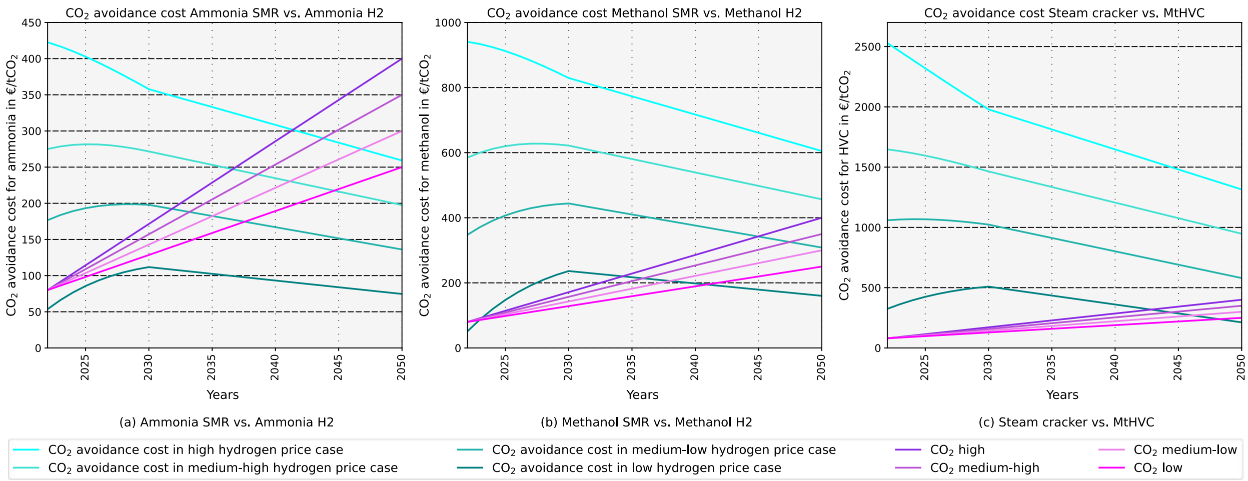

Fig. 6. CO_2 avoidance costs for chemicals (ammonia (a), methanol (b) and HVC (c)) production in the four different hydrogen price sensitivities and comparison to the four defined CO_2 price paths

to blast furnaces. For the lowest CO_2 and highest hydrogen price sensitivity, the switch from natural gas to hydrogen remains incomplete until 2050. In contrast, the share of H2-DRI increases drastically with increasing CO_2 prices and decreasing hydrogen prices according to the avoidance cost curves from Figure 5 (c) up to nearly 100% diffusion of hydrogen-based processes.

Higher CO_2 prices also accelerate the diffusion of hydrogen-based ammonia production. However, in case of the high hydrogen price sensitivity, even with the highest CO_2 price path, hydrogen only supplies about 50% of the entire plant stock. The remaining plants already reinvested in (SMR) using natural gas, which are assumed to operate for 25 years. Lower hydrogen prices lead to earlier and higher shares of hydrogen-based ammonia production of up to nearly 80%.

For MtHVC and climate-neutral methanol, the high and medium-high hydrogen price paths prevent hydrogen diffusion, even with high CO_2 prices. Climate-neutral methanol shows low shares of 15-30% by 2050 for the medium-low hydrogen price sensitivities and reaches 65% at low hydrogen prices. Similarly, low hydrogen prices start the slow diffusion of hydrogen-based HVC production, which reaches shares of 20 to 40% by 2050. Thus, conventional steam crackers persist until 2050 regardless of price variations due to the high demand for hydrogen and the low impact of the CO_2 price. Overall, comparing the diffusion dynamics shows that full market diffusion by 2050 is unlikely even under a broad range of economic assumptions if the natural reinvestment cycle remains unchanged. This is particularly valid for the chemical processes that switch from fossil feedstock to hydrogen and have a large proportion of the carbon embedded in the products.

To better understand these diffusion patterns, it's essential to examine reinvestments in fossil processes. Figure 8 compares the individual products for two selected sensitivities both showing a linear increase of the CO_2 price from 80 €/tCO_2 in 2022 to 300 €/tCO_2 in 2050: Sensitivity 5 (highest hydrogen price path: 57 €/GJ in 2022 to 30 €/GJ in 2050) and sensitivity 8 (lowest hydrogen price path: 27 €/GJ in 2022 to 15 €/GJ in 2050).

Figure 8 shows both the total production shares and new annual investment in tons per process. This illustrates the long-term effects of early reinvestments in fossil processes, which are still operating in 2050 thereby perpetuating a fossil-based production system. Fossil lock-in reinvestments are lowest for steel, although there are still a few investments in blast furnaces until 2031. These are, however, replaced by DRI in the second reinvestment cycle. The diffusion of H2-DRI depends strongly on the hydrogen price. While NG-DRI shows high shares until 2045 in sensitivity 5, the stock is dominated by H2-DRI from the beginning in sensitivity 8. For the basic chemical products, Figure 8 shows larger shares of fossil reinvestments. Sensitivity 5 is completely dominated by reinvestments in fossil processes, most of which operate until 2050. In comparison, sensitivity 8 shows substantial investments in climate-neutral processes due to its low hydrogen price path, with the highest market share for ammonia among the basic chemicals. However, there are still reinvestments in fossil SMR throughout the entire period until 2050. Here, the limited access to hydrogen infrastructure partly results in avoiding the use of hydrogen (see section 3.2.2).

For HVC, investments in fossil-based steam crackers dominate until 2050, with a few hydrogen-based MtHVC investments appearing mainly after 2045, resulting in a 20% market share. A similar trend is observed for methanol but ending in higher shares of climate-neutral production of around 60%. Across all products, the results indicate that the substantial share of investments required in the near future put considerable pressure on the industry.

For steel, around 90% of blast furnace capacity requires relining between 2025 and 2040. In the basic chemicals plant stock, 41% of steam cracker capacity, 22% of ammonia capacity and 51% of methanol capacity will reach their end of life before 2030. Thus, policy makers need to quickly establish an economic framework that encourages a switch to climate-neutral processes. Bridging processes like NG-DRI, which significantly reduce CO_2 emissions, enable a transition to climate-neutral hydrogen once it becomes available at competitive prices and avoid fossil lock-ins.

3.2.2. *Regional resolution and hydrogen transport infrastructure*

Figure 9 illustrates the spatial distribution of all considered plants. The size of each bubble represents the cumulative energy demand across all energy carriers at each site in 2022. HVC sites have the highest consumption due to high feedstock use, followed by primary steel sites, ammonia, and methanol. Northwest Europe, including western Germany, the Netherlands and Belgium shows the highest density of industrial plants and energy demand. Central and eastern Europe also have a comparatively dense heavy industry landscape compared to the north and south. Appendix F shows the spatial and temporal development of the energy demand for each energy carrier for sensitivity 16. Hydrogen demand and its distribution are limited by infrastructure constraints and the plans of the EHB consortium. Early industry transformation towards hydrogen use starts in the region including western Germany, the Netherlands and Belgium at primary steel manufacturing sites and some ammonia plants by 2030. By 2040, primary steel transformation is nearly complete, expanding towards the eastern Europe and

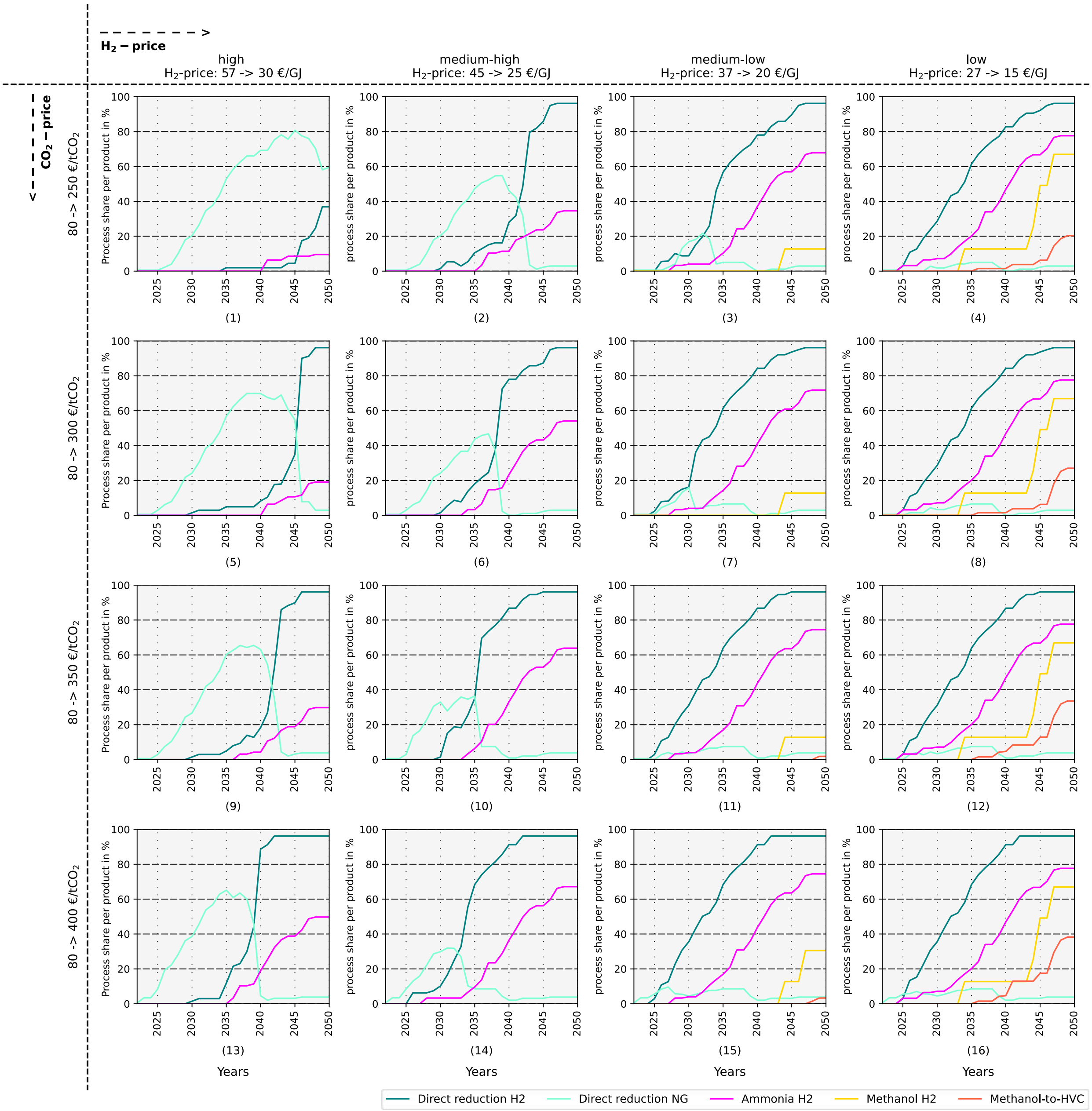

Fig. 7. Share of total production per process depending on hydrogen and CO_2-prices (Fig. 3).
Hydrogen prices variate per column according to defined price paths from Fig. 3 ***(a)****.* CO_2*-prices variate per row according to defined price paths from* Fig. 3 ***(b)***

the first HVC and methanol plants start operating with hydrogen. Between 2040 and 2050, several HVC plants are replaced by MtHVC, in line with a strong increase in hydrogen use across Europe as well as an almost complete substitution of ammonia plants.

Figure 10 compares sensitivity 16 (a) with a variation where investment behaviour is not restricted by the consideration of hydrogen infrastructure (b). The spatial and process-related difference (c) indicates that hydrogen-based processes are not chosen at some sites because of the missing connection to hydrogen infrastructure, especially in Scandinavian countries and France.

In southern Italy, HVC sites must make investment decisions before accessing hydrogen infrastructure (d), leading to fossil production lock-ins. For a total of 16 sites, the absence of hydrogen infrastructure when investment decisions are made increases the likelihood of fossil re-investments. The other plants not investing in hydrogen-based processes until 2050 are stuck in lock-in investments for economic reasons.

3.3. *Impacts of market diffusion*

Following, the impact of the market diffusion and switch towards hydrogen-based processes on the energy demand, and more specifically the hydrogen demand as well as corresponding investments and emission mitigation are analysed.

3.3.1. *Energy demand*

The diffusion of hydrogen-based processes dependent on hydrogen

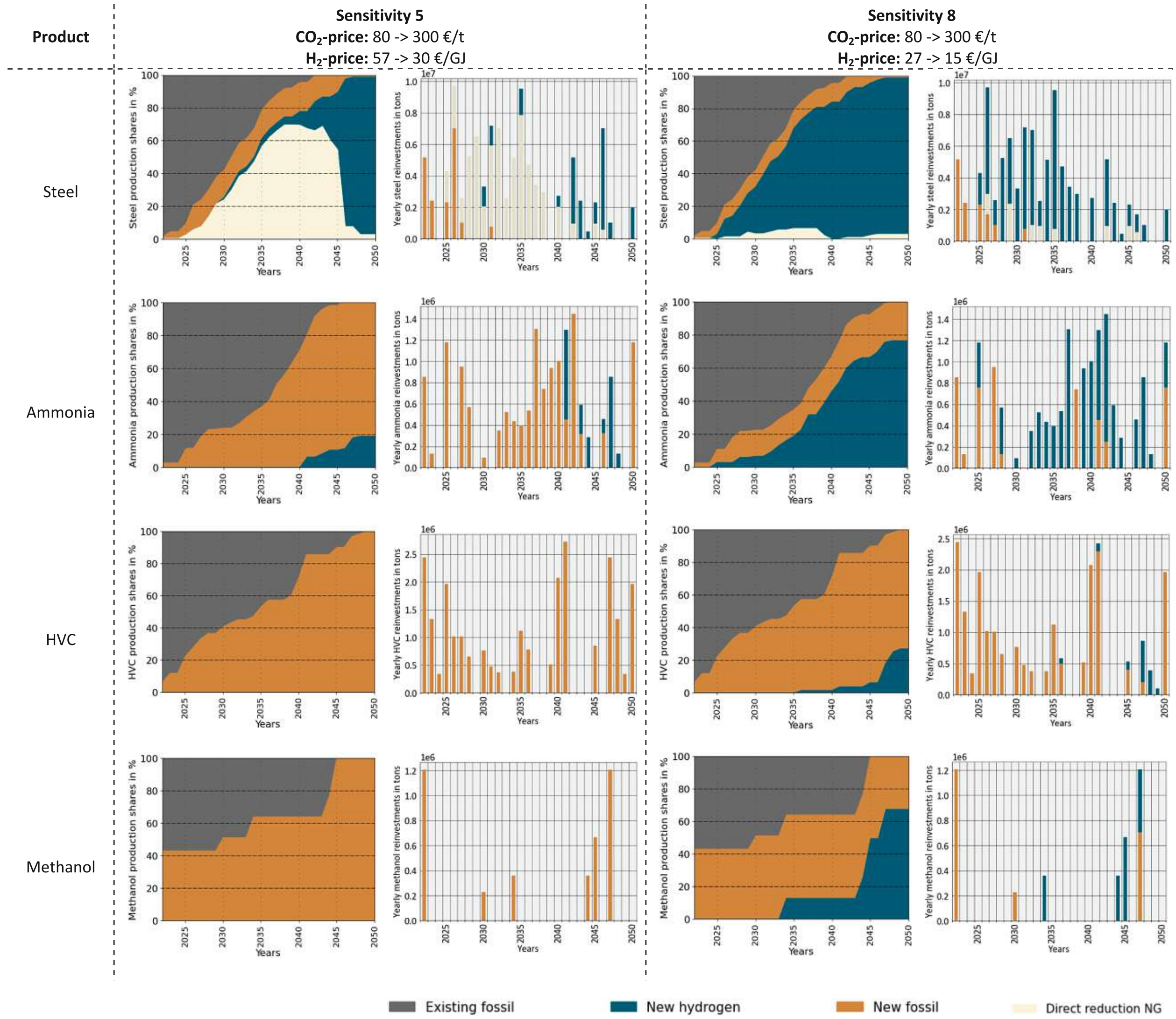

Fig. 8. Total production capacity and annual new investments by product and process

and CO_2 prices leads to varying energy demand per energy carrier in the sensitivities.

In 2022, coal (23%), natural gas (27%) and naphtha (42%) dominate the final demand, including feedstock, in EU27+3 for the considered products. Based on the share of total production per process from Figure 7, the sensitivities in Figure 11 shows that low CO_2 prices and high hydrogen prices result in high natural gas usage, no decrease in naphtha, and minimal hydrogen use for a few ammonia plants and H2-DRI by 2050. However, these conditions still lead to a complete phase-out of coal use in blast furnaces, as NG-DRI is competitive.

The higher the CO_2 price and the lower the hydrogen price, the more the share of natural gas decreases over time and is replaced by hydrogen. This effect is driven by the economic shift from NG-DRI to H2-DRI and the increasing hydrogen use for ammonia production. Hydrogen as a feedstock for HVC production is only able to compete with naphtha at very low hydrogen prices, as the CO_2 price has a limited effect due to the comparatively small quantities of natural gas used energetically in steam crackers. High CO_2 prices and low hydrogen prices in Germany make MtHVC competitive from late 2043 (Figure 6 (c)), resulting in early lock-in investments. Despite optimistic assumptions, substantial amounts of natural gas (~150 TWh) and naphtha (~ 50 TWh) remain in 2050.

Overall, the final energy demand decreases in all sensitivities, mainly as a result from switching in primary steel production to DRI process, which consumes less energy than blast furnaces. Using hydrogen in DRI is more efficient than using natural gas, so higher shares of H2-DRI further reduce final energy demand in primary steel production. The detailed development for single products and countries is provided in the supplementary material.

3.3.2. *Diffusion of hydrogen demand per product*

None of the conducted sensitivities leads to a complete adoption of hydrogen-based processes for all products (Figure 7). However, hydrogen demand varies significantly by factor 8, ranging from 64 TWh to 507 TWh.

Figure 12 indicates that a higher CO_2 price and a lower hydrogen price trigger an earlier hydrogen ramp-up and increasing shares of hydrogen until 2050. The penalty from CO_2 prices on the emissions from the energetic use of natural gas in steam crackers is insufficient to achieve market diffusion of the MtHVC process at medium to high hydrogen prices. Low naphtha prices and the ineffectiveness of the CO_2

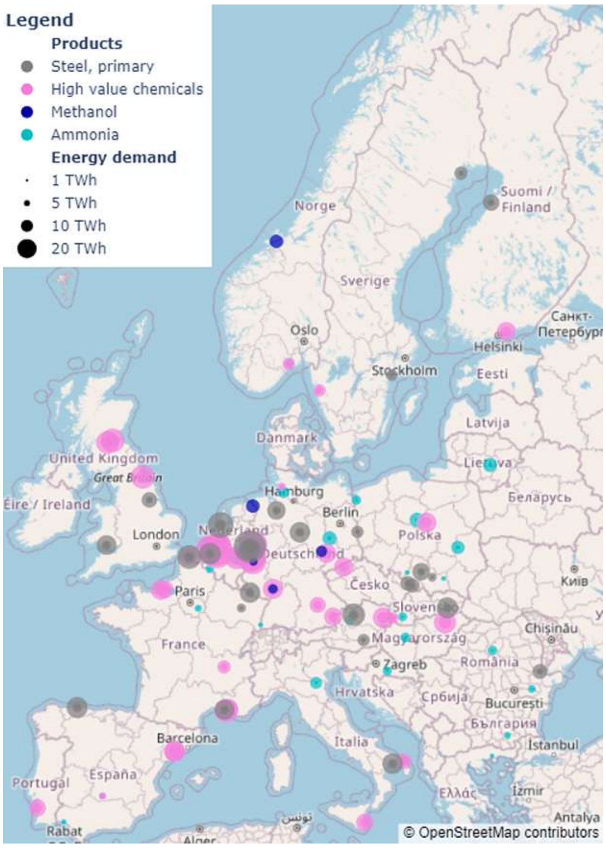

Fig. 9. Locations of primary steel, HVC, ammonia and methanol plants in Europe sized by their current final energy demand.

price on fossil feedstock consumption lead to economic advantages for fossil steam crackers However, for low hydrogen and high CO_2 prices, 20 of the 47 HVC plants may reinvest in MtHVC and these account for about 280 TWh of total hydrogen demand in 2050. This indicates that the EU's future hydrogen demand is highly sensitive to development and investment decisions in HVC production, if no intermediates like methanol or other synthetic energy carriers are imported for these purposes. If all steam cracker plants adopted the MtHVC process, total hydrogen demand could reach around 1000 TWh.

3.3.3. Investments

The analysis of total investments per process in Figure 13 shows the expected outcome based on the production shares from Figure 7. The need to reinvest for blast furnaces follows a roughly linear trend and leads to investment decisions for around 70% of all primary steel plants until 2037.

Low CO_2 prices and high hydrogen prices provoke earlier process switching in primary steel plants and substantial investments in NG-DRI, which is, however, flexible in using hydrogen instead of natural gas. Interestingly, high CO_2 prices trigger more early investments in NG-DRI than low CO_2 prices. The higher CO_2 prices trigger early NG-DRI investments instead of blast furnace relining, which leads to a higher share of DRI in the early years. The second major investment block is the renewal of the EU's steam cracker plants. Some older steam cracker plants require early investment, and a second huge investment phase starts from 2035 onwards. Even with very low hydrogen and high CO_2 prices, investments in MtHVC only become attractive compared to conventional steam crackers around 2040 at the earliest. This is when more than 50% of the conventional steam cracker plants already required reinvestment based on their typical lifetime. All sensitivities also show lock-in investments for ammonia and methanol plants, as the hydrogen and CO_2 prices make hydrogen-based production economically unattractive or hydrogen from the EHB is not available in time.

Overall, the investments in ammonia and methanol production are nearly negligible compared to those in primary steel and HVC production. For ammonia, only small investments for ASU and Haber-Bosch adjustments are necessary, as hydrogen is expected to be supplied via pipeline. Methanol has only small capacities in the EU27+3 and specific investments are lower than for primary steel or HVC plants.

3.3.4. Greenhouse gas emissions

Low CO_2 prices and high hydrogen prices contribute to the continued use of coal through reinvestments in conventional blast furnaces and an increased reliance on natural gas in NG-DRI and chemicals production, as depicted in Figure 14. Thus, for low CO_2 and high hydrogen prices, emissions are only reduced by 10% until 2030 and by 55% until 2050. Higher CO_2 prices lead to a faster phase-out of coal and its related

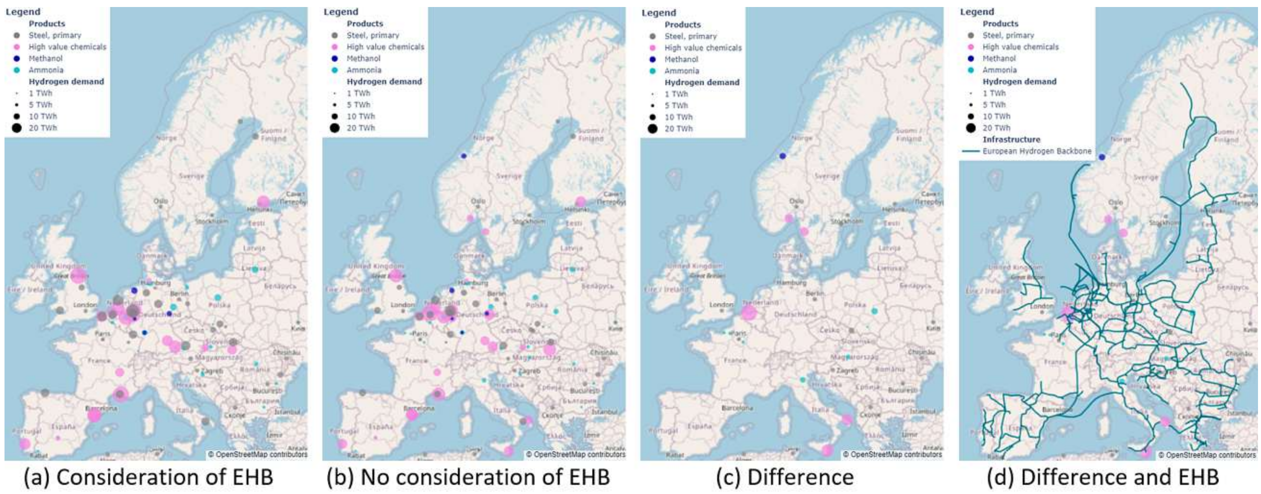

Fig. 10. Spatial distribution of the resulting hydrogen demand of sensitivity 16 in 2050 considering the dependence on hydrogen infrastructure according to EHB plans (a), without considering the availability of hydrogen infrastructure for the investment decision (b), and the difference in hydrogen demand and its spatial distribution without (c) and with (d) displaying the respective infrastructures.

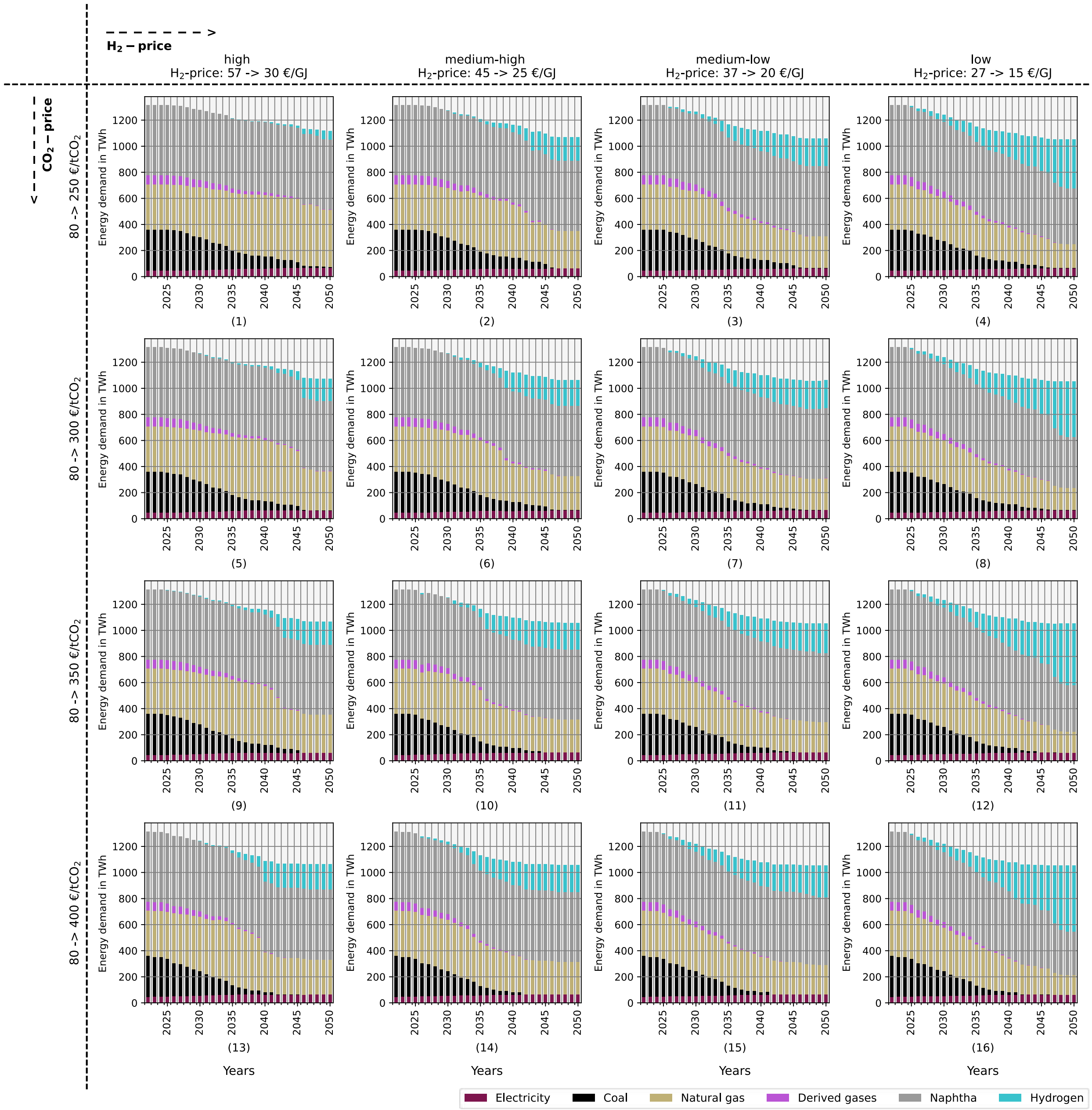

Fig. 11. Share of final energy demand (including feedstock demand) depending on hydrogen and CO_2 prices (Fig. 3).

emissions, while lower hydrogen prices have a smaller effect on the early replacement of blast furnaces. However, lower hydrogen prices do lead to the earlier substitution of natural gas as an energy source and therefore lower emissions. In general, high CO_2 prices lead to an almost complete phase-out of coal use until 2043, while process-related emissions from DRI and natural gas use in steam crackers account for 16% in the most optimistic sensitivity.

Thus, the reduction of energy-related CO_2 emissions varies between 55% and 84% in the sensitivity analyses.

4. Discussion

4.1. Potential role of other mitigation options

While this paper focuses on the framework needed for hydrogen-based processes, other mitigation options like electrification, CCU/S, or biomass will certainly also play a role in the future decarbonisation of the steel and chemicals industries [63]. These were not included in the quantitative modelling but are discussed here. Applying CCU/S at blast furnaces could mitigate CO_2 by only 20-40% [64]. When making retrofit investments for top gas recycling blast furnaces, capture rates may be improved up to around 50-70% [65]. While the costs for the emitted CO_2 would decrease with higher capture rates, additional costs for the

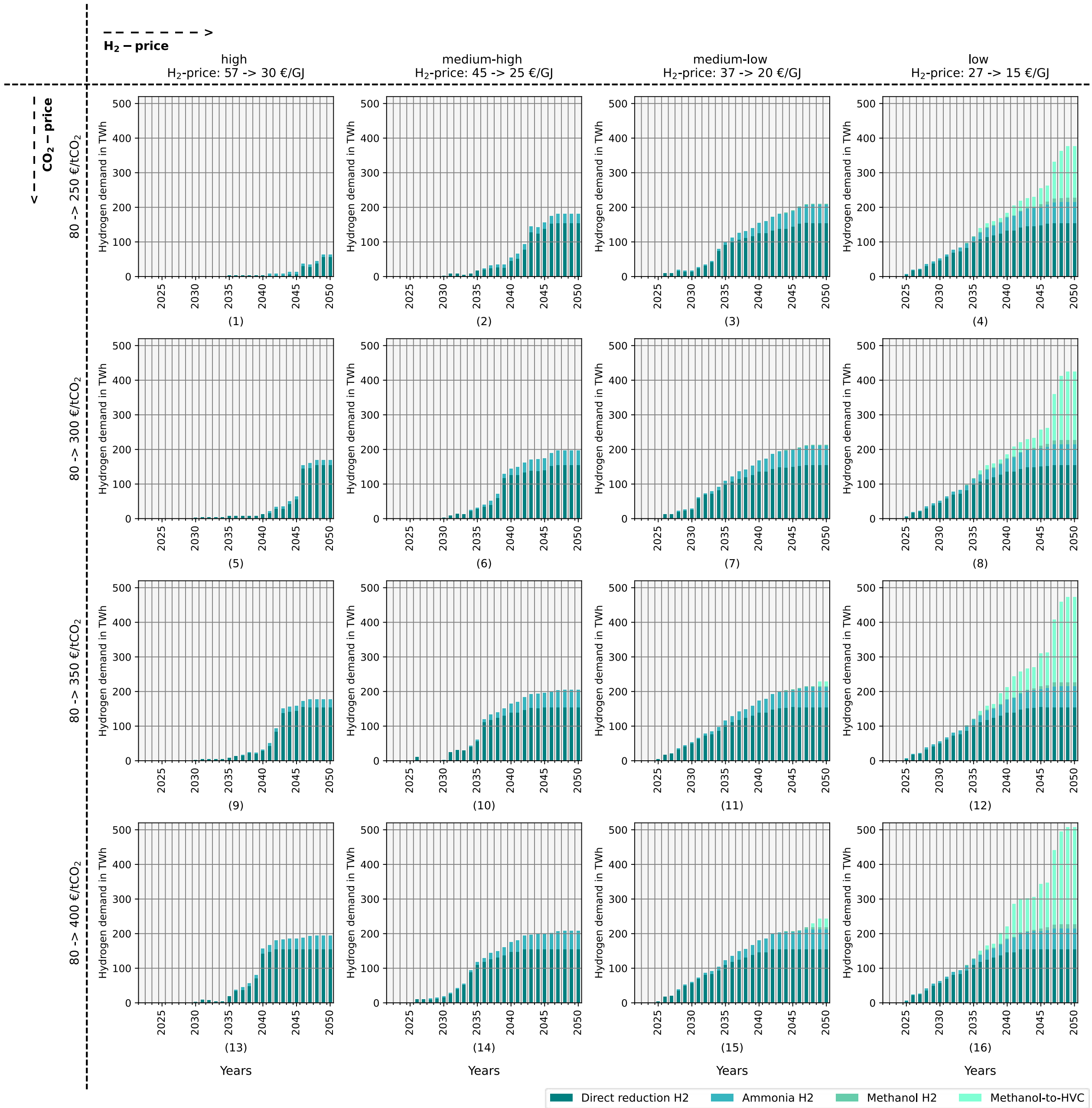

Fig. 12. Share of hydrogen demand per product (including feedstock demand) depending on hydrogen and CO_2 prices (Fig. 3).

capture technology and energy are required and remaining emissions would need to be compensated [66]. Direct electrification of primary steel production is currently not technically mature and unlikely to play a significant role in the near future [67]. Secondary steel production is limited by scrap availability but is likely to increase in the future as it is much more energy-efficient than primary production. This would reduce the potential demand for H2-DRI. However, even if the above options emerge, H2-DRI is still reckoned to be the major technology for future clean steel production [68], also because industry has already made decisions in this direction. Most European steel projects focus either on hydrogen or electrification [69]. Reviews on clean primary steel production also show huge activities in Europe and Asia [70].

CCU/S is also an option for ammonia production [71]. Some of the CO_2 produced is already being captured and utilised today at individual sites with integrated urea production [72]. Similar to blast furnaces, it is not possible to capture all the emissions and additional investments in CCU/S technology, transport and storage or use would be needed. Electrochemical options like solid state ammonia synthesis are not yet technically mature or cost-competitive [73].

Research on electrifying steam cracker furnaces is ongoing, but the technology is still in its early stages and its large-scale integration remains uncertain [74]. Once available on industrial scale, it might be competitive using synthetic climate-neutral feedstock in the long-term.

The production of HVC and methanol requires a carbon source, currently provided by fossil fuels. In the transition to hydrogen-based processes, CO_2 will therefore play an important role [75]. The analysis

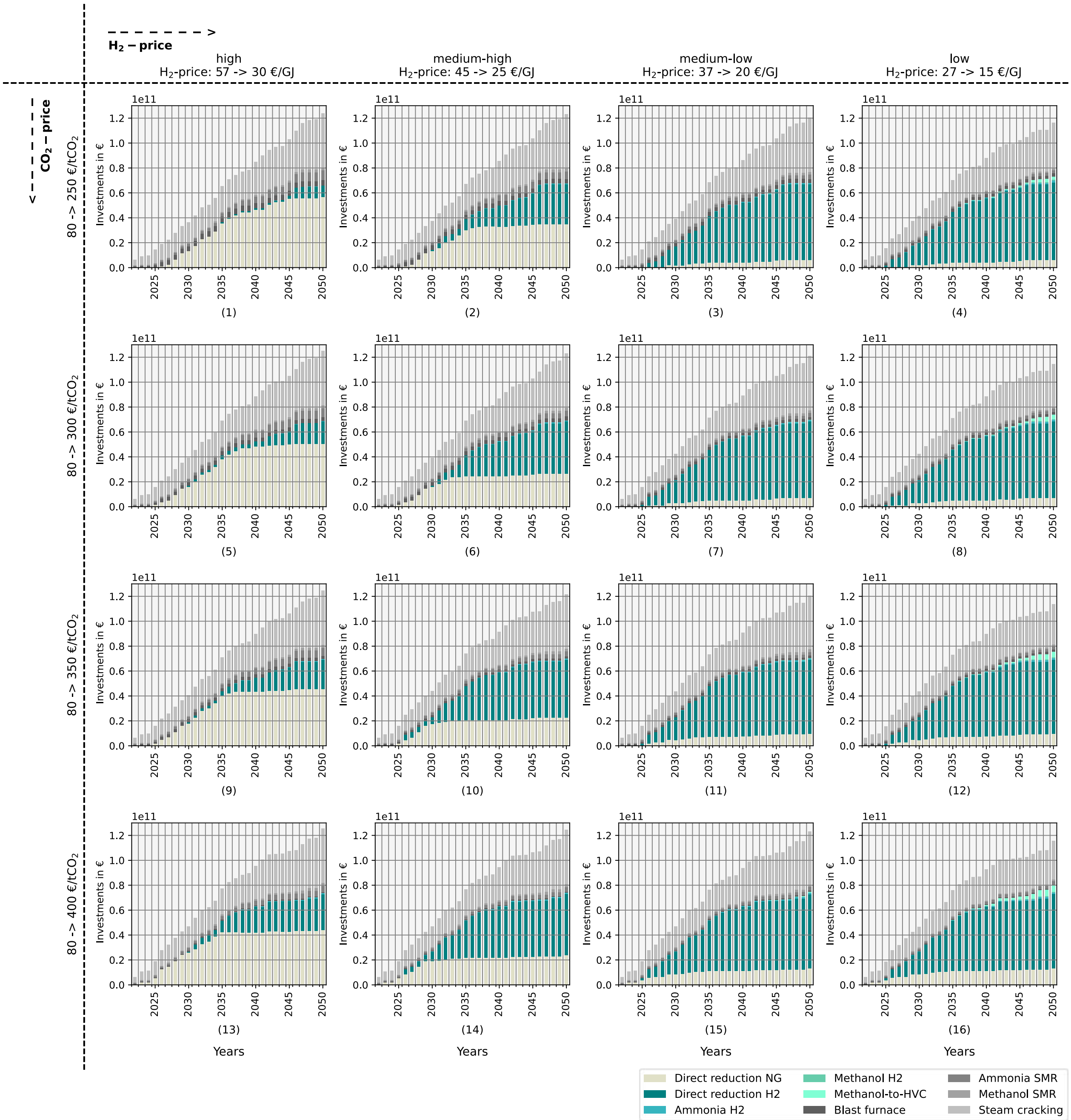

Fig. 13. Total investments per process due to process switch depending on hydrogen and CO_2 prices (Fig. 3).

does not specify the carbon source for methanol and HVC production via MtHVC, but hard-to-abate process-related emissions from cement or lime production could serve as a carbon source, possibly reducing costs in CO_2 emitting branches [76]. Waste incineration plants, included in EU ETS regulations from 2028 [77], will face economic pressure to avoid CO_2 emissions, with captured CO_2 either stored or used in industry. However, using fossil emissions as carbon feedstock necessitates closed carbon cycles or compensation to ensure climate neutrality [78]. Another often discussed option is direct air capture, though potentially more expensive, can achieve large-scale negative emissions. Current unclear boundary conditions and a lack of planning for CO_2 storage and infrastructure make the future of CCU/S or other possible value chains difficult to predict. There are hardly any detailed plans or a regulatory framework for dealing with CCU/S at present, but it is important to closely consider the interplay between a hydrogen and carbon economy. In February 2024, the European Commission released a first draft towards an industrial carbon management that aims to establish a cooperation platform, identify demand, and promote corresponding value chains. [79]. Biomass as a feedstock for basic chemicals is another option, but its availability may be insufficient to transform the entire chemical industry [80].

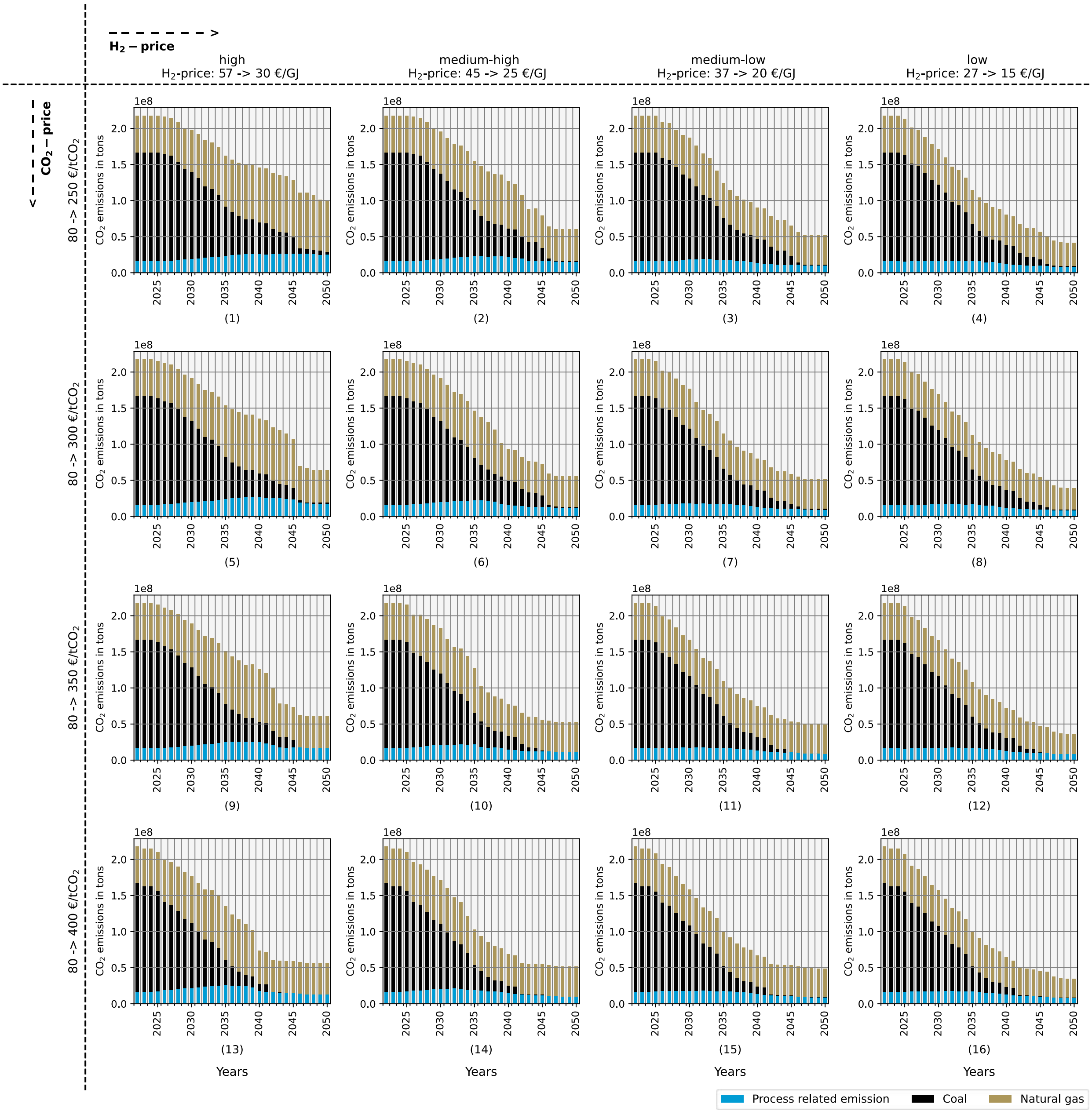

Fig. 14. Total emissions due to process switch depending on hydrogen and CO_2 prices (Fig. 3).

4.2. *Effect of CO_2 pricing*

The results show that NG-DRI becomes competitive with fossil blast furnaces for steel production, assuming CO_2 opportunity costs are considered in investment decisions and neglecting benchmarking. This indicates the significant role of NG-DRI in the transition and synergies with developing a hydrogen system. Among others, the conversion of ammonia production could be one of the beneficiaries of DRI and infrastructure investments. With hydrogen infrastructure access, direct hydrogen use becomes economically viable over time compared to syngas from SMR. The analysis follows the current definition of EU ETS for the effect of CO_2 pricing, considering only direct emissions (scope 1) [30]. Especially for HVC, the assumed range of CO_2 prices is insufficient to make hydrogen-based feedstock competitive, as large amounts of fossil naphtha as a feedstock (scope 3) are not affected by the CO_2 price. Additional measures, such as blending quotas for synthetic aviation fuels (SAF) [81], subsidies for green energy sources, or a CO_2 tax on feedstock, will be necessary to address high fossil fuel consumption. Furthermore, demand-side policies promoting green lead markets could stimulate the transition to climate-neutral feedstock. It is crucial to consider the role of imports, their future development, origin, and corresponding regulation and labelling in this context.

4.3. *Reflection of plant ages and average lifetimes*

The key drivers for technology diffusion in this modelling approach are the age distribution of the current plant fleet and the resulting typical average reinvestment cycles. However, assuming major reinvestments is always a simplification of reality; sites can be partially modernised, or reinvestments postponed. Reinvestment cycles are less accurate for chemical products than for primary steel production due to regular maintenance, modernisation and incremental improvements to increase efficiency and avoid downtime [82]. In addition, the lower temperatures compared to steel lead to longer material lifetimes in chemical plants. Theoretical lifetimes for basic chemicals should therefore be seen more as modernisation cycles rather than reinvestment cycles. However, these modernisation costs still account for high cost shares [83] and can determine the decision for new investments.

For primary steel production, reinvestments are more discrete, making this approach is more accurate [41]. Despite uncertainties in distinct reinvestment cycles, older plants generally require more reinvestment and modernization than newer ones, validating the use of reinvestment cycles to capture such patterns. The results show that basically each plant has one large investment decision until 2050 to avoid lock-ins [84].

4.4. *Structure of global value chains*

The shown variations on future hydrogen demand from 64 to 507 TWh occur from the uncertainties in future hydrogen prices and depend on economic factors. Early reinvestments (e.g. driven by additional external factors like policies) before the end of a plant's lifetime could increase hydrogen demand from the investigated 64 to 507 TWh in the sensitivities up to 1000 TWh for the considered products [18]. However, the analyses reflect today's industry structure and value chains within Europe, without considering potential restructuring of global value chains, such as importing intermediate or end products. Prioritising different processes or establishing alternative value chains could lead to different developments. Recent studies have started to consider importing intermediate products, such as hot briquetted iron (HBI) for primary steel production [85]. In case of restructured value chains for the investigated products during the transition, it is essential to verify the robustness of hydrogen quantities and transport requirements to effectively construct a European hydrogen infrastructure. Other studies have already indicated the need for cross-country transport without drawing conclusions about individual pipelines or detailed changes in capacity [86].

4.5. *The need for hydrogen infrastructure*

The commissioning timelines for the individual hydrogen pipelines of the EHB initiative fit the calculated upcoming investments for most of the industry sites considered. For some sites illustrated in Figure 10, the planned commissioning year for the hydrogen pipelines could be too late or the pipeline is not close enough thus leading to lock-in investments in this analysis. Small shifts in the timing of investment decisions or adjustments to the plans for EHB could address this.

This alignment is expected for large industrial clusters, but the situation may differ for other sectors and smaller sites. These include the production of glass, ceramics, cement, lime, and metal products, which could all potentially use hydrogen to decarbonise production processes. Future research should extend the approach used in this paper to additional sectors beyond the major steel and chemical sites.

4.6. *Summary*

To achieve a sustainable transformation of the industry, it is essential to integrate infrastructure planning, the restructuring of global value chains, and circularity within the framework of a carbon and hydrogen economy. Various other barriers to industry decarbonisation have been identified and discussed alongside existing policies in the literature [87]. These interconnected aspects necessitate comprehensive consideration and further research to understand the hurdles of industry decarbonisation. Here, a broad range of hydrogen price developments from literature had been used to investigate on the diffusion of hydrogen-based processes in the considered industry branches. This work and the developed approach can contribute to assessing decarbonisation options and transformation pathways. The insights and data provided can serve as basis for further research in energy system analysis and suitable policy measures.

5. Conclusions

Many studies expect industry to become the main hydrogen consumer in the future, although there is still substantial uncertainty about the dynamics and concrete pathways. This paper investigates the spatial and temporal dynamics of technology diffusion for primary steel, ammonia, HVC, and methanol using a plant-specific simulation model. The model considers the existing European plant stock and includes their georeferenced location, individual plant ages, production capacities, and reinvestment cycles. Investment decisions are based on overall production costs, comparing hydrogen-based and fossil-based processes.

The analysis reveals that for all plants considered at least one investment opportunity remains until 2050, with 36% requiring reinvestment by 2030 and 58% by 2035. Only few might have a second reinvestment opportunity. The results indicate significant pressure on industry to reinvest in fossil processes. For steel, 90% of blast furnaces need relining between 2025 and 2040. For HVC, 41% of steam crackers will reach their end of life before 2030. Policymakers must create an economic framework supporting climate-neutral processes. This early need for reinvestment poses a high risk of locking in fossil fuel-based processes before climate-neutral hydrogen supply can be established. Bridging processes like NG-DRI, which reduce CO_2 emissions immediately and later switch to hydrogen, should be exploited to avoid fossil lock-ins.

To understand the impact of economic factors, 16 defined sensitivities vary hydrogen and CO_2 prices. The results show that the economic competitiveness of climate-neutral processes heavily depends on hydrogen prices, which are uncertain. However, the economic viability also varies strongly among the products and processes. Hydrogen-based alternatives for methanol and HVC are not cost-competitive in the medium term and require low hydrogen prices as CO_2 prices have a weak impact as most carbon is embedded in products rather than emitted during production. Enhancing the competitiveness of climate-neutral processes to produce HVC, methanol and ammonia is substantial in the short and medium term to avoid reinvestments in fossil-based processes. For steel, the combination of a high CO_2 price impact on coal-fired blast furnaces and the availability of transitional natural gas-based direct reduction of iron ore (NG-DRI) mitigates the risk of fossil lock-ins. Full market diffusion by 2050 across the products is unlikely if natural reinvestment cycles remain unchanged, especially for chemical processes switching from fossil feedstock to hydrogen.

Assuming that the structure and spatial distribution of European industry remains similar to today, the highest hydrogen demand will be in Northwestern Europe, including Germany, the Netherlands and Belgium. Sensitivity 16, which shows the highest hydrogen demand, shows around 39 TWh for 2030 and 229 TWh for 2050 in those regions out of 64 TWh for 2030 and 507 TWh for 2050 in EU27+3, respectively. These estimates consider plant ages, reinvestment cycles and infrastructure availability, but not specific investment plans or government subsidies. However, the market diffusion remains incomplete, and the total technical potential is about 1000 TWh in the EU27+3, assuming constant production volumes.

The plant-specific market diffusion is calculated in dependence of hydrogen infrastructure according to the EHB with a proximity of 30 km. Only 16 sites will require reinvestment before the planned hydrogen infrastructure is operating or have no access within this proximity.

Here, hydrogen-based processes are examined in isolation. Future research should consider and analyse the competition with alternative climate-neutral processes like direct electrification, biomass or carbon capture, especially for those plants without access to hydrogen infrastructure. In addition, a better understanding is required of potential changes in value chains, including imports of intermediate energy-intensive products [88], or the renewables pull effect [89], and this calls for investigations from a global perspective. In addition, the approach can be used next to assess how well the planned hydrogen or other infrastructure fits the needs of other energy-intensive industries like glass, ceramics or metal processing.

CRediT authorship contribution statement

Marius Neuwirth: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Tobias Fleiter:** Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization. **René Hofmann:** Writing – review & editing, Supervision, Resources, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Most important data (model input, industry site information, result files) are shared as supplementary material as open data. Any further data will be made available upon request.

Acknowledgements

This research was carried out as part of the TransHyDE project, grant number 03HY201L, and we gratefully acknowledge the funding provided by the German Federal Ministry of Education and Research (BMBF). Parts of this work was also conducted within the TRANSIENCE project, grant number 101137606, funded by the European Commission within the Horizon Europe Research and Innovation Programme.

We thank Gillian Bowman-Köhler for native spell and grammar check.

Financial support

This work was financially supported by the German Federal Ministry of Education and Research in the context of the 'TransHyDE' project, grant number 03HY201L. Parts of this work are also related to the TRANSIENCE project, grant number 101137606, funded by the European Commission within the Horizon Europe Research and Innovation Programme.

Appendix A:. Process diffusion model

The behaviour of technology diffusion in industry differs from other areas where known diffusion theories try to reflect socio-economic behaviour. For example, the long life cycles and very high investments involved in industry lead to very specific points of time for reinvestment. Furthermore, bad investments entail an enormous risk in terms of loss of economic competitiveness. In most cases, energy costs account for the biggest proportion of total production costs (TCOP). Apart from economic aspects, aspects like the availability of energy carriers and the corresponding infrastructure also determine investment decisions in industry. On the other hand, investment decisions in industry are much more rational and cost-benefit based than they are for consumers. To sum up, technology diffusion in industrial stock is strongly dependent on the plant age and lifetime of current processes as well as the cost-effectiveness and competitiveness of the investment options.

Based on this context, the model initialises each industrial site. Investments in new processes are made according to reinvestment cycles calculated based on the specific age and process lifetime of each site. The industry sites decide separately for each plant which process is the most economic investment for the upcoming life cycle by comparing the TCOP of all alternatives (equation (1)). The alternatives can be limited depending on the availability of energy carriers in the respective region and distance to necessary infrastructure or by applying a technology ban.

$$Inv_p = \min(TCOP) \tag{1}$$

Inv_p process with lowest TCOP evaluated for new investment for the individual plant

$TCOP$ total cost of production (TCOP)

The total cost of production per process is calculated from the total specific production cost per process multiplied by the annual output of the plant (equation (2)).

$$TCOP = c_p \bullet o_{pu} \tag{2}$$

c_p specific production costs per process available per plant

o_{pu} output in tons of yearly production per production unit

The specific production cost represents the sum of different cost components per ton of product, comprising the annuity on investment, operational costs, energy-related costs and external influences like penalties for emissions as well as subsidies or funding (equation (3)).

$$c_p = c_a + c_o + c_{ec} + c_{ext} \tag{3}$$

c_p specific total cost per ton of product

c_a specific annuity on investment per ton of product

c_o specific operational costs per ton of product

c_{ec} specific energy carrier costs per ton of product

c_{ext} external influences on specific total cost per ton of product

Appendix B:. Number of sites and plants per country

Appendix B1 shows the detailed number of plants per product and process for each country.

There is additional information for all of these sites on company affiliation, geocoordinates, emissions and related plants on site level as well as production capacity, process and plant age on plant level. A more detailed resolution is provided in the supplementary material S1_2.

Appendix B1: Number of manufacturing sites and plants per product and process in Europe for basic chemicals and primary steel production per country covered in this analysis.

Country	Number of	Steel, primary		Olefins	Ammonia	Methanol	Sum
		BF/BOF	NG-DRI/EAF	Steam cracker	Steam reforming	Steam reforming	
AT	Sites	2		1	1		4
	Plants	5		1	2		8
BE	Sites	1		2	2		5
	Plants	2		3	2		7
BG	Sites				1		1
	Plants				1		1
CZ	Sites	2		1	1		4
	Plants	4		1	1		6
DE	Sites	7	1	9	4	4	25
	Plants	15	1	14	6	4	40
EE	Sites				1		1
	Plants				1		1
EL	Sites				1		1
	Plants				1		1
ES	Sites	1		3	2		6
	Plants	2		3	2		7
FI	Sites	1		1			2
	Plants	2		1			3
FR	Sites	3		6	4		13
	Plants	8		6	4		18
HR	Sites				1		1
	Plants				1		1
HU	Sites	1		1	1		3
	Plants	1		2	1		4
IT	Sites	1		2	1		4
	Plants	3		2	1		6
LT	Sites				1		1
	Plants				2		2
NL	Sites	1		3	1	1	6
	Plants	2		6	5	2	15
NO	Sites			1	1	1	3
	Plants			1	1	1	3
PL	Sites	2		1	5		8
	Plants	3		1	8		12
PT	Sites			1			1
	Plants			1			1
RO	Sites	1			2		3
	Plants	1			2		3
SE	Sites	2		1			3
	Plants	3		1			4
SK	Sites	1		1	1		3
	Plants	3		1	1		5
UK	Sites	2		3	3		8
	Plants	4		3	3		10
Sum	Sites	28	1	37	34	6	96*
	Plants	58	1	47	45	7	158

* Some of the chemicals plants are located at the same site. Thus, the number of sites in this table do not add up to 96 when counted separately.

Appendix B2 shows the manually derived sources for steam cracker plants.

Appendix B2: Sources from manual search for steam cracker plants

Country	Company	Website
General Information: https://de.wikipedia.org/wiki/Liste_der_Erd%C3%B6lraffinerien		
AT	OMV/Borealis	https://www.borealisgroup.com/company/history; https://www.omv.com/services/downloads/00/omv.com/1522207986091/dload_ir_Factbook2020_EN_DE
BE	TOA	https://totalenergies.com/media/news/press-releases/belgium-total-completes-the-upgrade-of-its-largest-refining-and-petrochemicals-platform-in-europe
BE	BASF	https://www.basf.com/global/images/about-us/history/BASF_Chronik_Gesamt_en.pdf.assetdownload.pdf; https://www.basf.com/be/en/who-we-are/Group-Companies/BASF-Antwerpen/About-the-site/History.html#accordion_v2-d72a3ed53c-item-cd0f64125b; https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/
BE	Sabic Europe	https://2b1stconsulting.com/sabic-invests-170-million-in-geleen-naphtha-cracker/
NL	Shell	https://www.shell.com/business-customers/chemicals/media-releases/2020-media-releases/shell-invests-in-new-furnaces-to-reduce-emissions-from-its-moerdijk-chemicals-plant.html; https://nl.wikipedia.org/wiki/Shell_Moerdijk; https://www.shell.com/business-customers/chemicals/media-releases/2014-media-releases/shell-moerdijk-40-years.html
BE	Dow	https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/

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(*continued*)

Country	Company	Website
CZ	Unipetrol	https://www.linde-engineering.com/en/about-linde-engineering/success-stories/rescue-plan-for-refinery.html; https://www.process.vogel.de/wie-linde-einen-zerstoerten-unipetrol-steamcracker-wieder-aufbaut-a-634912/; https://www.unipetrol.cz/en/AboutUs/Pages/History.aspx
FI	Borealis	https://www.borealisgroup.com/company/history; https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/; https://www.omv.com/services/downloads/00/omv.com/1522207986091/dload_ir_Factbook2020_EN_DE
FR	LyondellBasell	https://www.lyondellbasell.com/en/about-us/history/; https://new.societechimiquedefrance.fr/wp-content/uploads/2021/05/b_9_000_000.vf3-sav.pdf
FR	Versalis	https://de.wikipedia.org/wiki/Liste_der_Erd%C3%B6lraffinerien
FR	A.P. Feyzin	https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/
FR	Total	http://www.beyond3d.com.au/uploads/9/1/6/8/9168625/035.pdf; https://totalenergies.com/system/files/documents/2022-03/DEU_21_VA.pdf
FR	Naphtachimie	https://new.societechimiquedefrance.fr/wp-content/uploads/2021/05/b_9_000_000.vf3-sav.pdf
FR	ExxonMobil	https://de.wikipedia.org/wiki/Liste_der_Erd%C3%B6lraffinerien
DE	Dow	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	OMV/Borealis	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	BP	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	Klesch	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	Ineos Olefins	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	BASF	https://www.basf.com/global/images/about-us/history/BASF_Chronik_Gesamt_en.pdf.assetdownload.pdf; https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	LyondellBasell	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
DE	Shell	https://epub.wupperinst.org/frontdoor/deliver/index/docId/7067/file/7067_Low-carbon-Industrie.pdf
HU	MOL	https://molgroup.info/en/our-business/downstream/production-sites
IT	Versalis	https://www.chemanager-online.com/en/news/petchems-age-porto-marghera-may-really-end
NO	Ineos Olefins	https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/
PL	PKN Orlen	http://abarrelfull.wikidot.com/plock-refinery; https://en.wikipedia.org/wiki/P%C5%82ock_refinery
PT	Repsol	https://www.ordemengenheiros.pt/fotos/editor2/regiaosul/oe_repsol_polimeros_site_21nov2018.pdf
SL	MOL	https://molgroup.info/en/our-business/downstream/production-sites
ES	Repsol	https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/; https://www.k-online.com/en/Media_News/News/Repsol_restarts_its_Tarragona_cracker_1
ES	Dow	https://digital.library.mcgill.ca/images/hrcorpreports/pdfs/6/636970.pdf; https://www.spglobal.com/pdf/RW2014-13-toc_214324110917062932.pdf; https://ekj-co.com/wp-content/uploads/2022/12/REFERENCE-LIST-2019-Nacional.pdf; https://ence.uz/Reference_list_2012.pdf
SE	Borealis	https://www.borealisgroup.com/company/history; https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/
UK	Ineos Olefins	https://www.chemistryworld.com/news/grangemouth-will-switch-to-shale-gas-feed-by-2016-says-ineos/7223.article; https://en.wikipedia.org/wiki/Grangemouth_Refinery
UK	ExxonMobil	https://www.exxonmobil.co.uk/News/Newsroom/UK-News-releases/2019/0917_ExxonMobil-announces-further-investment-at-Fife-Ethylene-Plant; https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/
UK	Sabic UK	http://www.mrcplast.com/news-news_open-395021.html; https://www.cgfi.ac.uk/spatial-finance-initiative/geoasset-project/petrochemicals/; https://www.sabic-teesside.co.uk/en/teesside-site/wilton-site; https://www.icis.com/explore/resources/news/2021/10/28/10699571/sabic-s-wilton-uk-cracker-to-restart-after-850m-investment-could-run-on-hydrogen/

Appendix B3 shows the manually derived sources for ammonia plants.

Appendix B3: Sources from manual search for ammonia plants.

Country	Company	Website
General Information: https://eippcb.jrc.ec.europa.eu/sites/default/files/2019-11/lvic_aaf.pdf		
AT	Borealis Agrolinz Melamine	https://www.borealisgroup.com/about-us/history
BE	YARA Belgium	https://www.yara.com/siteassets/investors/057-reports-and-presentations/other/2020/production-capacities-by-segment-september-2020-pdf.pdf; https://www.yara.nl/fr-be/a-propos-de-yara/yara-tertre/information/
BE	BASF Antwerp	https://www.basf.com/be/en/who-we-are/Group-Companies/BASF-Antwerpen/About-the-site/History.html#accordion_v2-d72a3ed53c-item-cd0f64125b
CZ	ORLEN Unipetrol	https://www.unipetrol.cz/en/AboutUs/Pages/History.aspx; https://chemicalparks.eu/news/orlen-unipetrol-ammonia-production-modernization;
EE	OSTCHEM Nitrofert Estonia	http://www.ostchem.com/en/o-kompanii/proizvodstvo/nitrofert
FR	Borealis	https://www.borealisgroup.com/about-us/history
FR	Yara France	https://www.yara.fr/a-propos-yara/nos-implantations/
NL	OCI	https://www.annualreports.com/HostedData/AnnualReportArchive/o/oci_2017.pdf; https://www.pbl.nl/sites/default/files/downloads/pbl-2019-decarbonisation-options-for-the-dutch-fertiliser-industry_3657.pdf
LT	Achema Lithuania	https://www.achema.lt/history
PL	Grupa Azoty	https://www.researchgate.net/publication/295603303_New_plant_for_neutralization_of_nitric_acid_with_ammonia_in_Grupa_Azoty_Zaklady_Azotowe_Kedzierzyn_Operational_experience; https://tarnow.grupaazoty.com/en/the-company/about-the-company/history
RO	Chemgas	https://ji.unfccc.int/UserManagement/FileStorage/Q3MP4NY5EJCSUF28LTKGXR70Z9HWOA; https://www.enpg.ro/wp-content/uploads/2023/08/Decarbonising_Romanias_Industry_Policy_Paper_updated_EPG.pdf
RO	InterAgro	https://www.romania-insider.com/donau-chem-reopening-jun-2020; https://seenews.com/news/interagro-reopens-donau-chem-fertilizer-plant-in-southern-romania-704511; https://www.enpg.ro/wp-content/uploads/2023/08/Decarbonising_Romanias_Industry_Policy_Paper_updated_EPG.pdf
UK	Severnside	https://www.theconstructionindex.co.uk/news/view/4500-tonne-uk-ammonia-plant-dismantled-for-reassembly-overseas
DE	Ineos	https://www.ineoskoeln.de/unternehmen/herkunft/
DE	BASF	https://www.basf.com/se/en/media/news-releases/20201/10/p-21-355.html
DE	Yara	https://de.wikipedia.org/wiki/Yara-Werk_Brunsb%C3%BCttel
DE	SKW	https://www.skwp.de/unternehmen/unternehmensprofil/historie/; https://www.skwp.de/fileadmin/content/05_mediacenter/broschueren/umwelterklaerung/Aktualisierung-Umwelterklaerung_2017.pdf; https://www.uni-kiel.de/anorg/lagaly/group/klausSchiver/piesteritz1.pdf

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Country	Company	Website
DE	BP Gelsenkirchen	
HU	Nitrogenmüvek	https://www.nitrogen.hu/hu/nitrogenmuvek-idovonal; https://bbj.hu/business/industry/manufacturing/nitrogenmuvek-restarts-ammonia-production
PL	Grupa Azoty Pulawy	https://pulawy.grupaazoty.com/en/the-company/about-the-company/history/history-in-the-years#60-s
PL	Grupa Azoty Kedzierzyn	https://zak.grupaazoty.com/spolka/o-firmie/historia

Appendix B4 shows the manually derived sources for methanol

Appendix B4: Sources from manual search for methanol plants.

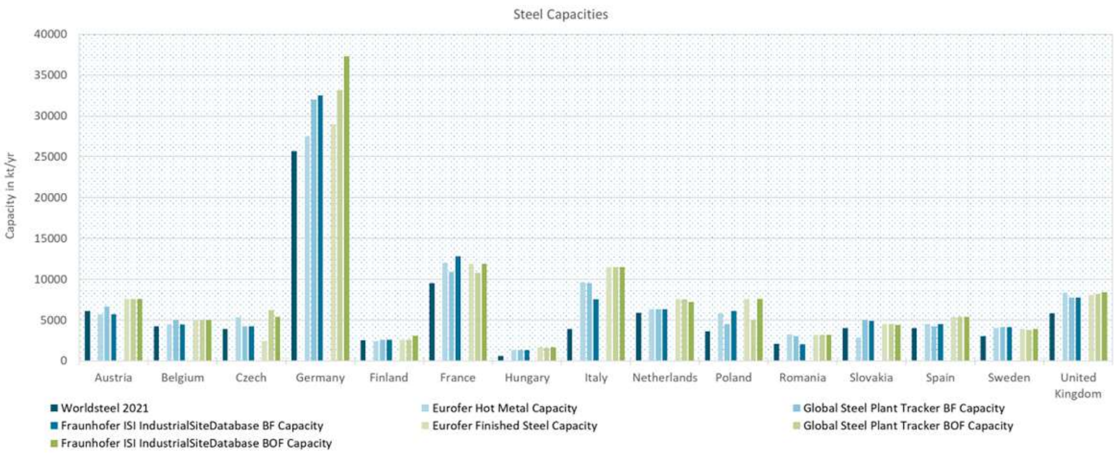
Country	Company	Website
DE	BASF	https://www.irena.org/-/media/Files/IRENA/Agency/Publication/2021/Jan/IRENA_Innovation_Renewable_Methanol_2021.pdf; https://www.basf.com/global/documents/de/about-us/history/History-in-Figures/1965-1989/1978_BASF_Geschaeftsbericht.pdf
DE	Total	https://www.deutsches-chemie-museum.de/datei/anzeigen/id/4131,1089/mb_11_1998_3_erdoel_schmierstoffe.pdf; https://www.mz.de/lokal/merseburg/spergau-leben-mit-der-raffinerie-2407613; https://www.process.vogel.de/richtfest-in-leuna-a-58386/
DE	Ruhr Oel	https://www.bp.com/de_de/germany/home/wo-wir-sind/raffinerie-gelsenkirchen/wer-wir-sind/zahlen-und-fakten.html; https://www.bp.com/content/dam/bp/country-sites/de_de/germany/home/unsere-raffinerien/raffinerie-gelsenkirchen/publikationen/ausgaben-2022/2022-12-gemeinsam-nachbarschaftszeitung.pdf
DE	Shell	https://s06.static-shell.com/content/dam/royaldutchshell/documents/corporate/manufacturing-rhinelandhistory.pdf
NO	Statoil	https://www.equinor.com/news/archive/202102-tjeldbergodden; https://www.tbu.no/en/ressurser/
NL	BioMCN	https://oci-global.com/news-stories/stories/oci-global-explores-sustainable-methanol-in-delfzijl/; https://www.irena.org/-/media/Files/IRENA/Agency/Publication/2021/Jan/IRENA_Innovation_Renewable_Methanol_2021.pdf

Appendix C:. Validation of industry site data

As an indicator, a comparison was made of the last complete and confirmed production quantities per product and country. Based on official sources, the completeness of production capacities of the developed Fraunhofer ISI IndustrialSiteDatabase for the products considered was validated.

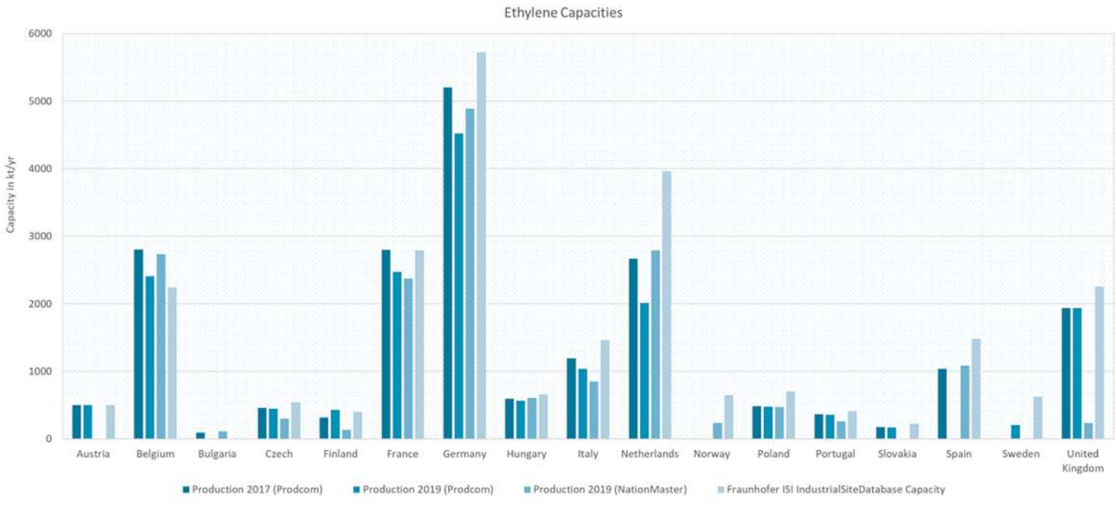
Primary steel capacities:

The World Steel Association [90] annually publishes national production volumes per product type and process, while Eurofer [32] and Global Steel Plant Tracker [33] serve as references for plant capacities of the iron and steel sector. **Appendix C 1** shows the comparison of the national production volume of pig iron from blast furnaces and the capacities of the above-mentioned sources and the Fraunhofer ISI IndustrialSiteDatabase. Overall, a very good match of plant capacities for blast furnaces and oxygen converters can be seen for all countries. This suggests a complete mapping of primary steel production for the modelling. Minor deviations between the sources can be validated by manual internet research on corresponding values of the database used for modelling.



Appendix C1: Primary steel production in 2021 [90] and comparison of primary steel capacities per country from Eurofer [32], Global Steel Plant Tracker [33] and Fraunhofer ISI IndustrialSiteDatabase

Ethylene capacities (representative for HVC):



Appendix C2: Ethylene production in 2017 and 2019 from Prodcom [37] and NationMaster [91] and comparison with national capacity from Fraunhofer ISI IndustrialSiteDatabase

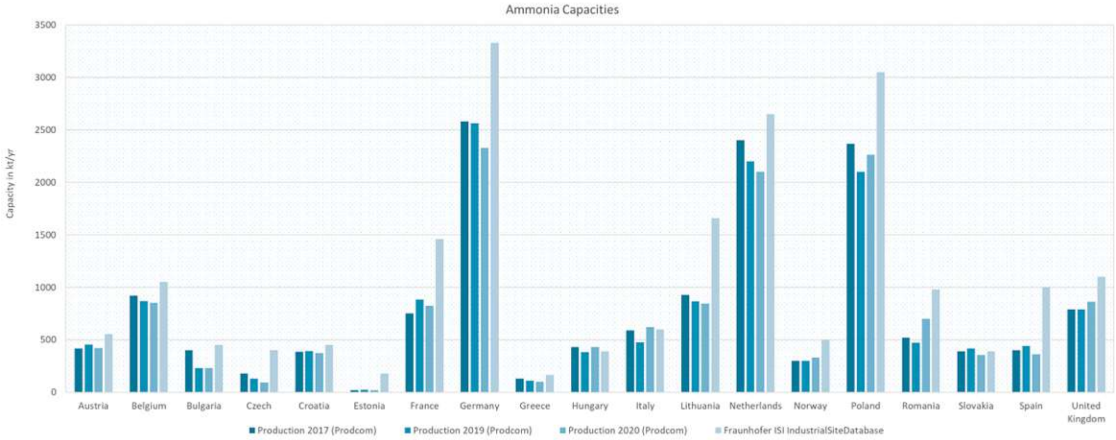
In general, the data for chemicals production are not as readily available as for the iron and steel sector. Furthermore, value chains in the chemical sector are more complex and it is therefore harder to understand and collect detailed and comprehensive data. In case of high value chemicals (olefins and aromatics), the largest shares are produced in steam cracker plants in Europe by cracking naphtha that serves as a fossil feedstock.

As there are no statistics from any international association, **Appendix C 2** displays the comparison of national production volumes per country for 2017 and 2019 from Prodcom [37] and NationMaster [91] and collected plant capacities within Fraunhofer ISI IndustrialSiteDatabase. However, especially for non-EU countries like Norway or the UK, it is difficult to gather information. Overall, the collected plant capacities match the respective national production and are complete for all the covered countries, with the exception of very small amounts in Bulgaria.

Ammonia capacities:

As already stated for HVC, gathering data on ammonia production plants in Europe was challenging in some cases. However, older grey literature and screening European chemical company websites led to a thorough dataset including information about plant age. As shown in **Appendix C 3**, comparing the annual production for 2017, 2019 and 2020 taken from Prodcom [37] with the data collected on production capacities indicates the completeness of Fraunhofer ISI IndustrialSiteDatabase. Comparing the geospatial resolution of the collected sites and plants also shows conformity with other reports [36].

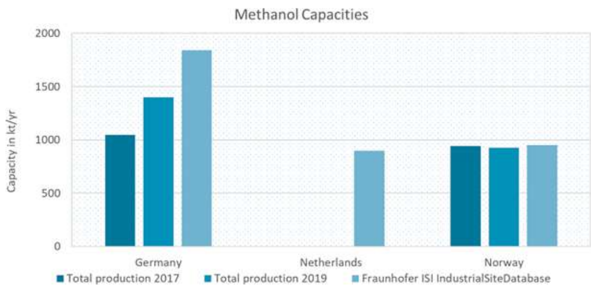
In a few cases (France, Germany, Lithuania, Poland, Spain), ammonia production capacity greatly exceeds production. This may result from direct urea production not being reported as ammonia manufacturing at specific sites in these countries or from low utilisation factors.



Appendix C3: Ammonia production in 2017, 2019 and 2020 from Prodcom [37] and comparison with national capacities from Fraunhofer ISI IndustrialSiteDatabase

Methanol capacities:

While methanol is seen as playing a major role as an energy carrier and feedstock in future industrial value chains [92], current production capacities in Europe are small. Germany, the Netherlands and Norway account for the majority of European production [37]. However, due to the monopoly of the companies involved, there is no obligation to report any official statistics. The methanol plant in Romania was closed in 2021. Despite these obstacles, **Appendix C 4** indicates the completeness of the Fraunhofer ISI IndustrialSiteDatabase for European methanol facilities.



Appendix C4: Methanol production in 2017 and 2019 from Prodcom [37] and comparison with national capacity from Fraunhofer ISI IndustrialSiteDatabase

Appendix D:. Model validation

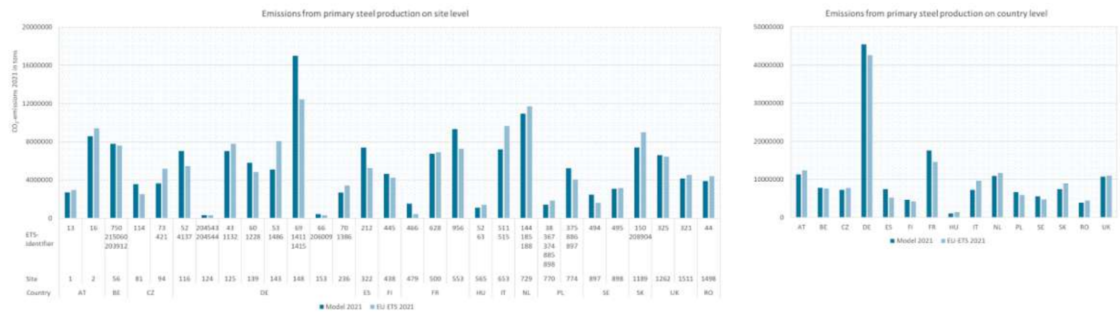
Apart from validating the data basis used for modelling, it is also crucial that model heuristics, calculations and results are reliable. However, validating such detailed data input and model results requires statistics of a similar granularity for comparison. Here, calibration of the plant-specific model input data is according to the production outputs presented in **Appendix C**. More precisely, to estimate the average production per plant, the national utilisation factor is applied per product, calculated by dividing the annual production by the available annual capacity per country. This assumption is simultaneously the restricting factor, which may lead to differences occurring between individual sites in each country, as it assumes a similar average load factor for each plant. Having calibrated the production output per plant, the modelled results of the calculated CO_2 emissions are compared with the emission reporting within the EU ETS [93] on a site and country-level for the respective year. The calculation within the model is based on the input data on the energy and steam demand per process and the corresponding shares of energy carrier use. The underlying emission factors (Table 3) for each energy carrier result in the calculated emissions per plant and site.

For the comparison, however, the level of detail for reported emissions in the EU ETS is not uniform. While some companies report one single value for all facilities at a site, others report individual values for each plant.

When comparing the results for the calculated emissions, indirectly also validation of the data and calculations of energy demand per energy carrier and other indicators is given, as these equations form the basis for the resulting plant-specific emissions.

Primary Steel:

For primary steel manufacturing sites, the site-level comparison is shown in **Appendix D 1** (a) for 2021. The averaged utilisation factor per plant leads to differences between individual sites for each country (e.g. site 143 and 148 in Germany), which indicates that they operated with a different capacity utilisation. When aggregating those results to a country level (**Appendix D 1** (b)), the calculated national emissions are a good match to the reported emissions within the EU ETS [93]. An exact match is neither expected nor manageable, as each plant differs in efficiency, degree of modernisation as well as process integration at large industry sites. Therefore, the aim is to reflect a realistic average, which can be proven and validated by these analyses. As the reporting within EU ETS also shows large inconsistencies, other installations had to be included in this comparison to allocate the facilities to the sites.



(a) (b)

Appendix D1: Comparison of calculated emissions from primary steel production based on national production in 2021 from the model calculation and reported EU ETS emissions [93] per site (a) and country (b)

Ammonia:

When comparing the calculated emissions from ammonia production with EU ETS facilities, some plants cannot be covered as they are part of refinery sites or chemical parks that do not report at facility level. **Appendix D 2** shows the comparison of the model results with identifiable emissions of single ammonia facilities as reported in the EU ETS. Steam methane reforming (SMR) with the respective techno-economic assumptions serves as a reference process for ammonia production in the model. As this process also covers the majority of ammonia plants operating in Europe, the emission comparison is a good match for most of the identified plants. However, larger differences occurred for individual plants, which can be explained by the fact that some use heavy oil to produce the required synthesis gas. The use of heavy oil results in higher energy demand as well as higher emission factors and around 30% higher emissions compared to SMR used as the reference process in the model. Especially for Germany and Lithuania, this seems to explain the differences.

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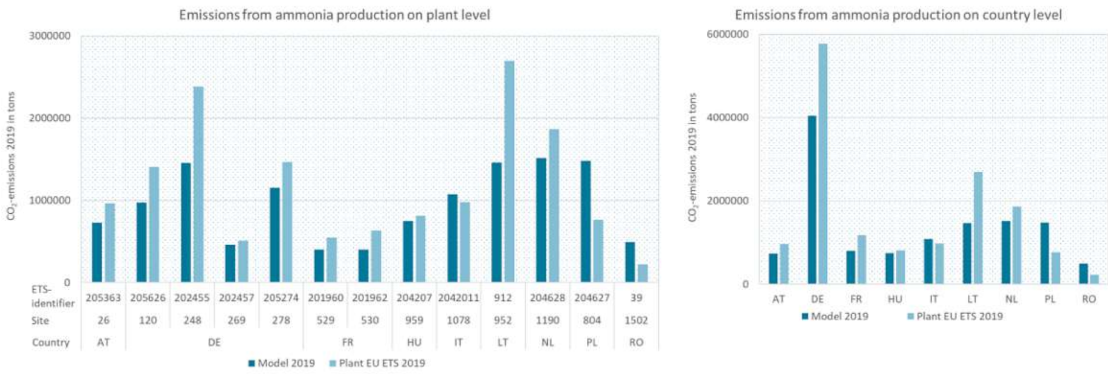
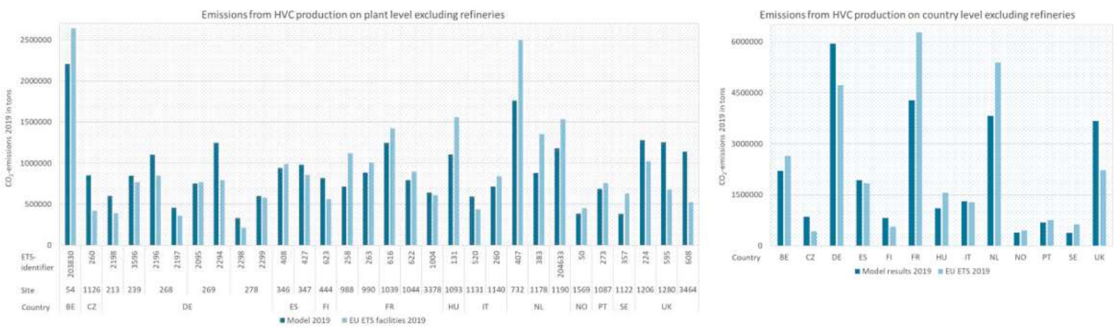


(a) (b)

Appendix D2: Comparison of calculated emissions from ammonia production based on national production from 2019 from the model calculation and reported EU ETS emissions [70] per site (a) and country (b)

Olefins:

Similar to ammonia plants, steam crackers for HVC production are partly located in huge chemical parks or refineries and are therefore not reported individually within the EU ETS. Refineries, in particular, do not report with a detailed resolution. Therefore, **Appendix D 3** shows a comparison excluding refinery sites. Steam cracking of naphtha is used as the reference process in the model for the techno-economic assumptions, which represents the most widely used process in Europe [94]. However, there are also uncertainties for HVC regarding the feedstock used and the degree of process integration within sites, e.g. for using excess heat. These uncertainties lead to some huge differences between sites and countries. Different plant ages, efficiencies, level of site integration and the utilisation factor applied mean that an exact match was not expected for individual plants and sites, but the comparison shows that the model results are validated within the expected variation.

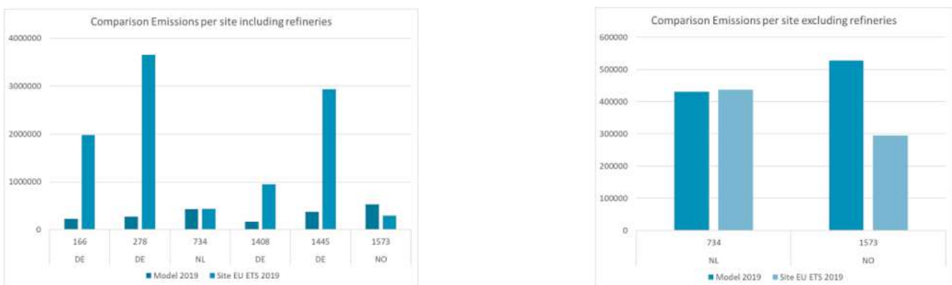


(a) (b)

Appendix D3: Comparison of calculated emissions from HVC production based on national production from 2019 from the model calculation and reported EU ETS emissions [70] per site (a) and country (b)

Methanol:

Methanol plants in Europe are mostly integrated in large refineries and not reported in the EU ETS as individual facilities, which results in enormous differences at site level (**Appendix D 4** (a)). The plants in the Netherlands and Norway are the exceptions. There is a good match with the emissions of methanol production in the Netherlands, while larger differences can be seen for the plant in Norway (**Appendix D 4** (b)). This could be explained by the use of biomass, for which emissions are not reported under the EU ETS, or the capture and re-use of CO_2 or the use of different feedstock, as SMR is taken as a reference for the production of synthesis gas in the model.

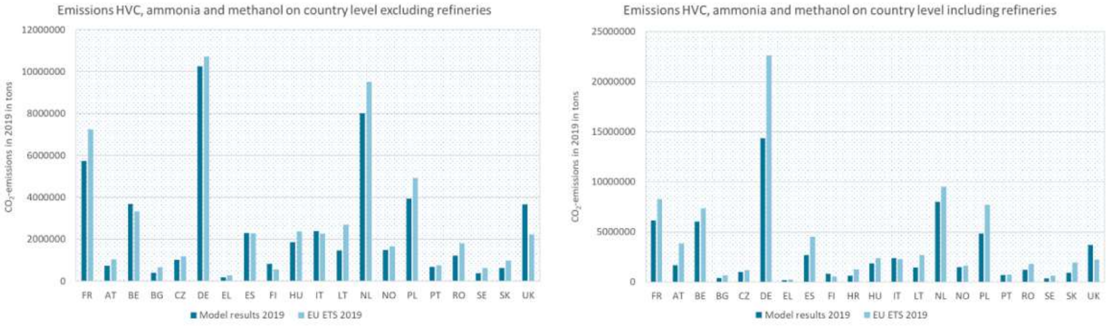


(a) (b)

Appendix D4: Comparison of calculated emissions from methanol production based on national production from 2019 from the model calculation and reported EU ETS emissions [70] per site (a) and country (b)

Chemicals total:

When comparing the emissions for HVC, ammonia and methanol calculated by the model with those reported in the EU ETS, there is a good match for aggregated national figures excluding refinery sites (**Appendix D 5** (a)) with relatively few deviations for each country. Germany, in particular, has comparably many steam cracker, ammonia and methanol plants located at refinery sites and this leads to an underestimation of their emissions by around 30% when including the whole emissions from refinery sites from EU ETS into the comparison.



(a) (b)

Appendix D5: Comparison of calculated emissions from chemicals production based on national production from 2019 from the model calculation and reported EU ETS emissions [70] per site (a) and country (b)

Appendix E:. Evaluation of reinvestment cycles

Uncertainties in anticipating reinvestment cycles arise from the site-specific and technical individuality of plants as well as the decision making of their owners concerning reinvestments and incremental improvements. Different types and scopes of measures to extend lifetimes also lead to postponed reinvestments that are difficult to anticipate. Thus, using theoretical reinvestment cycles based on statistics may deviate from the real-life point of investment. However, this approach draws a clearer picture of the possible transition pathways than the statistical diffusion theories used so far, especially due to the inclusion of the spatial component.

Primary steel (Blast furnaces):

Major reinvestment cycles in primary steel production are predetermined by the blast furnace campaign life. Renewal of the refractory lining and cooling units is crucial within such a relining. The literature often states lifetimes of 15-25 years for blast furnaces [40]. An analysis by Vogl et al. [41] estimated the correlation between the number of furnace campaigns and the resulting campaign lifetime. They calculated the median historical lifetime to be 17 years, and that the technical lifetime has increased in recent decades. Thus, the assumed lifetime is set to 20 years for retrofit in blast furnaces. Newly installed DRI plants have an estimated lifetime of 20-30 years and an average lifetime of 25 years is assumed in this study [43].

HVC (Steam cracker):

Steam crackers in many cases are very old plants that have undergone a variety of incremental investments and improvements with regard to higher efficiency, process integration, capacity increases and others. For this reason, it is difficult to assign them a lifetime. The figures in the literature range from an analysis period of 20 years [74] and lifetimes up to 30 [95] and 70 [96] years, depending on individual properties, degree of modernisation and number and type of incremental investments. However, the depreciation period and amortisation are often estimated as even shorter with 20 years in most cases [48]. In this study, an investment decision is assumed for each modernisation cycle of 25 years.

Ammonia (Steam reforming):

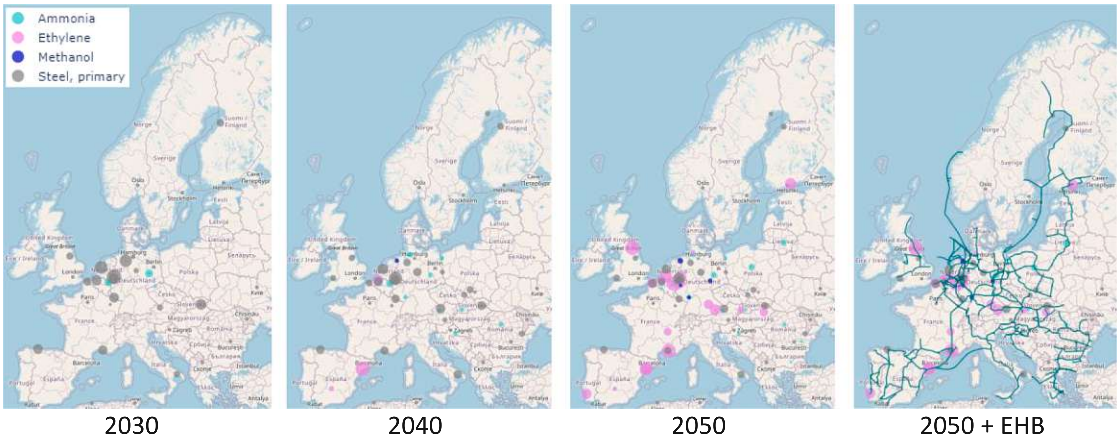
Ammonia production plants basically consist of two process steps: synthesis gas generation and a Haber-Bosch reactor to synthesize ammonia. The limitation to the technical lifetime results from the unit generating the synthesis gas as a Haber-Bosch reactor is stated to have long operating lifetimes of 40 [97] up to 50 [98] or even 60 [42] has an of 40-60 years, which can be prolonged by additional incremental investments. Steam methane reformers are most commonly used to supply the synthesis gas and have an economic and technical lifetime of 20 [99] to 30 [100] years. As the CO_2 emissions result from conventional synthesis gas generation, ammonia production can be decarbonised by substitution with green hydrogen and an air separation unit for nitrogen extraction. For these reasons, the assumed average lifetime of 25 years is set for reinvestment decisions on ammonia plants [101].

Methanol (Steam reforming):

Similar to ammonia, methanol production can also be separated into two process steps. First, synthesis gas generation to supply hydrogen and a carbon source, and second, the synthesis unit to produce methanol. A choice has to be made between process alternatives regarding the provision of the synthesis gas, as several alternatives are available. Conventional steam methane reformers or partial oxidation units for crude oil or coal compete with the external supply of hydrogen and CO_2 from biomass or other renewable sources. The assumed technical and economic lifetime is based on the literature and set to 25 years [102].

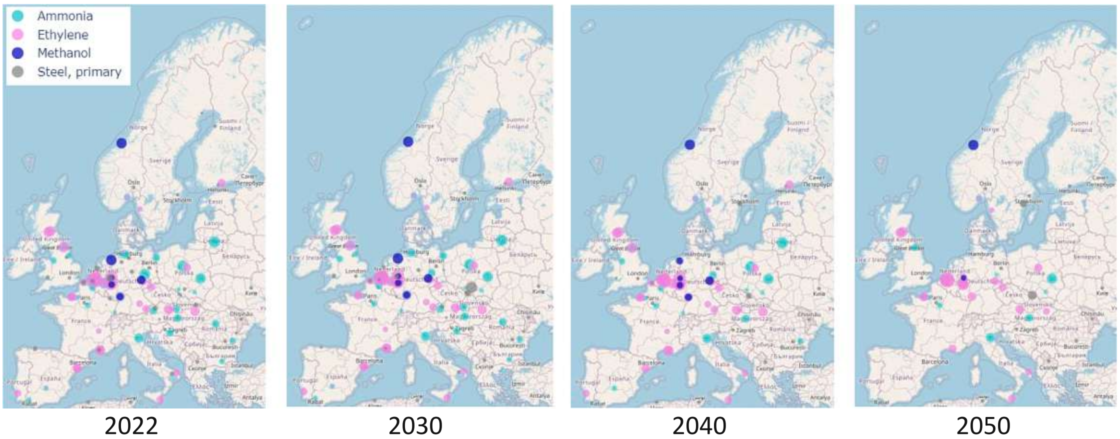
Appendix F:. Development of hydrogen, natural gas, naphtha and coal demand

Hydrogen demand:



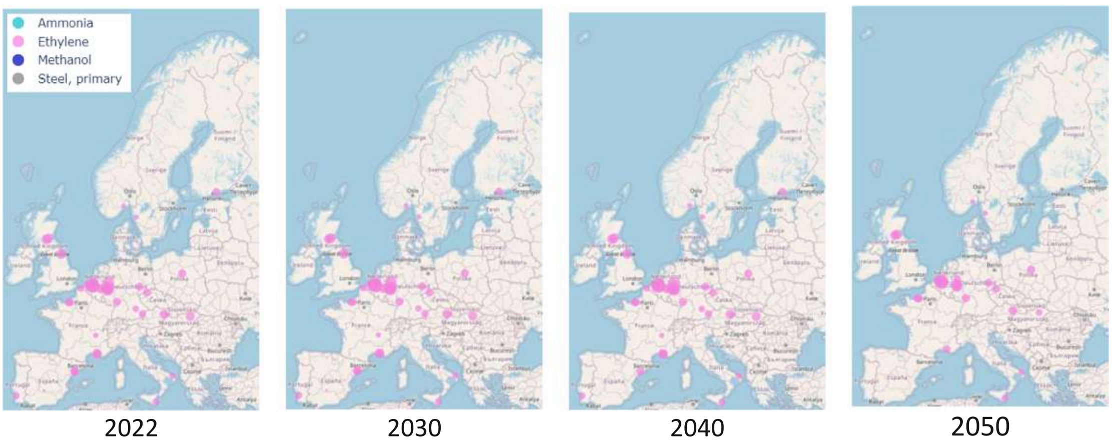
Appendix F1: Spatial development of hydrogen demand per product over time for low hydrogen and high CO_2 price sensitivity

Natural gas demand:



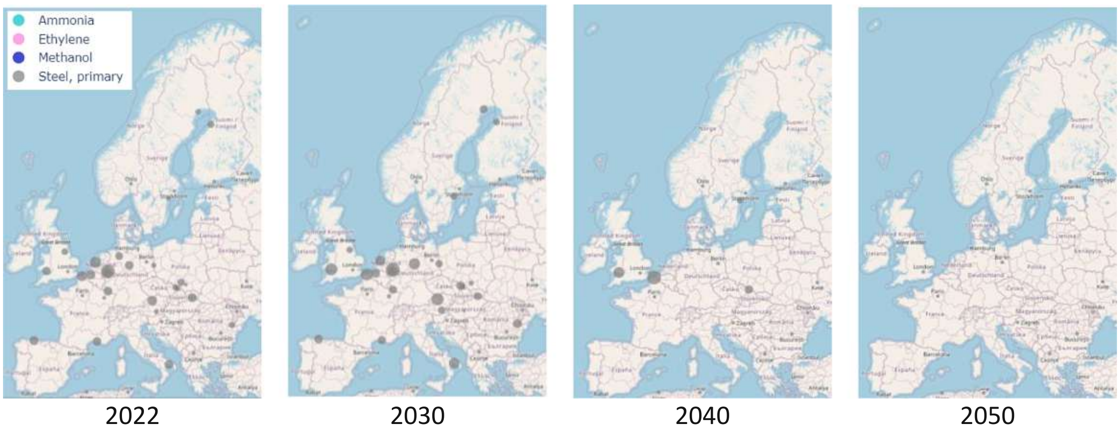
Appendix F2: Spatial development of natural gas demand per product over time for low hydrogen and high CO_2 price sensitivity

Naphtha demand:



Appendix F3: Spatial development of naphtha demand per product over time for low hydrogen and high CO_2 price sensitivity

Coal demand:



Appendix F4: Spatial development of coal demand per product over time for low hydrogen and high CO_2 price sensitivity

Supplementary material/supporting information

We provide extensive Excel files containing the result tables of the figures presented in this paper and additional very detailed information at country level. Further data or insights into the model will be made available on request.

S1: Model input data and assumptions

S1_1: The excel file transparently shows the techno-economic model inputs

S1_2: Total list of modelled industry sites with their properties

S2: Further detailed model results

S2_1: Final energy demand at country level for sensitivity 16 (4_400)

S2_2: Specific costs and their components per process for Germany for sensitivity 16 (4_400)

S2_3: Yearly total costs and their components for steel production and for all 16 sensitivities

S2_4: Yearly total costs and their components for ammonia production and for all 16 sensitivities

S2_5: Yearly total costs and their components for HVC production and for all 16 sensitivities

S2_6: Yearly total costs and their components for methanol production and for all 16 sensitivities

S2_7: Yearly total hydrogen demand and its components for all 16 sensitivities

S2_8: Cumulative investments and their components for all 16 sensitivities

S2_9: Yearly total emissions and their components for all 16 sensitivities

For some of the variables we had to focus on single countries or sensitivities for the supplementary material provided in this paper. Not all derived data can be made available due to the large quantity involved (more than 2000 Excel sheets). However, data for other sensitivities (in the case of S2_1) or other countries (in the case of S2_2) will be made available on request.

Appendix G. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.enconman.2024.119117.

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Further publications and other scientific contributions

Parts of my research connected to this thesis were not only published in the presented core publications but were the subject of other dissemination activities. These contributions are listed in this section.
This section is split into two kinds of further publications:

1. First, two additional main author conference articles, which were peer-reviewed and are listed in scopus, are presented (Papers I & II).
2. Second, two co-author journal publications (Papers A & B) and three peer-reviewed co-author conference articles (Papers C, D & E) and their contribution to this dissertation is summarised.

For all of those additional publications, a brief description is given, highlighting the most important findings in the context of this thesis. Additionally, my contribution to the main and co-author publications is explicitly presented.

Paper I – Main author conference publication

Hydrogen technologies for a CO_2-neutral chemical industry – a plant-specific bottom-up assessment of pathways to decarbonise the German chemical industry

This conference paper presents first attempts of investigating on process options for decarbonising chemical industry. Hydrogen, produced from renewable electricity, is essential in transitioning the chemical industry to a CO_2-neutral production. Considering the age structure of the existing German chemical plants, the transition to hydrogen-based processes could be faster than previously assumed. By 2030, 33% of basic chemical process installations in Germany can be replaced, and 89% by 2050. This transition would require substantial investments, estimated at 26 billion euros in capital in total and 15 billion euros in annual operating costs. The industrial sector in Germany is a major contributor to greenhouse gas emissions and relies heavily on fossil fuels. However, the successful implementation of hydrogen technologies depends on the availability of renewable electricity and the development of necessary infrastructure for electricity or hydrogen transportation. In summary, hydrogen has the potential to significantly reduce emissions in the industrial sector, but achieving this will require coordinated efforts in technology development, infrastructure, and policy support.

My contribution: Conceptualisation, Methodology, Validation, Formal Analysis, Data Curation, Writing - Original Draft & Editing, Visualisation.

M. Neuwirth & T. Fleiter (2020). "Hydrogen technologies for a CO2-neutral chemical industry – a plant-specific bottom-up assessment of pathways to decarbonise the German chemical industry". In: Eceee industrial summer study proceedings *2020-September*.
DOI: *10.24406/publica-fhg-409076*.
URL: *https://www.scopus.com/inward/record.uri?eid=2-s2.0-85137185498&partnerID=40&md5=aa85181feb4be0d712e61d6707a2b1c6*

Paper II – Main author conference publication

Future hydrogen demands from industry transition towards 2030 - a site-specific bottom-up assessment for North-Western Europe

This conference paper presents first attempts on establishing the method of the process diffusion behaviour of hydrogen-based processes in industry transition towards climate-neutrality. Based on the method and results from Paper 1 the Fraunhofer ISI IndustrialSite-Database was applied for the north-west European countries. An enhancement with plant ages and typical lifetimes enabled a first simple approach to determine possible diffusion pathways, but neglecting techno-economic information. Comparing and merging of the Fraunhofer ISI IndustrialSiteDatabase with the MIDDEN database represents another step of validation. References are calculated representing the potentials for specific applications. While Reference 1 reflects the maximum hydrogen potential for all identified applications covered site-specifically, Reference 2 excludes low-temperature heat applications, which could also relatively easy directly electrified. Reinvestment cycles based on plant age and typical process lifetimes are considered based on the definition of Reference 2 to assess a possible diffusion of hydrogen-based processes in 5-year steps. Those results are visualised and provided as open data: https://isi.pages.fraunhofer.de/eu-industry-transition/
North-west Germany and Belgium are identified to show the highest potential in the covered regions with 20 to 25 TWh of hydrogen demand each until 2030. First plans from the European Hydrogen Backbone initiative (EHB) to ramp-up hydrogen transport infrastructure are subsequently qualitatively compared to the results. Possible bottlenecks were identified in northern France and north-west Germany, where such first plans of a hydrogen infrastructure would have been late according to the theoretical reinvestment cycles.

My contribution: Conceptualisation, Methodology, Validation, Formal Analysis, Data Curation, Writing - Original Draft & Editing, Visualisation.

M. Neuwirth, M. Khanra, T. Fleiter, M. Jovicic & M. Shinde (2022b). "Future hydrogen demands from industry transition towards 2030 - a site-specific bottom-up assessment for North-Western Europe". In: Eceee Summer Study Proceedings.
DOI: *10.24406/publica-207*.
URL: *https://www.scopus.com/inward/record.uri?eid=2-s2.0-85178594122&partnerID=40&md5=f75840674517236ddb4e41c5fde76ef6*

Paper A – Co-author journal publication

Decarbonizing District Heating in EU-27 + UK: How Much Excess Heat Is Available from Industrial Sites?

P. Manz, K. Kermeli, U. Persson, M. Neuwirth, T. Fleiter, and W. Crijns-Graus (2020). "Decarbonizing District Heating in EU-27 + UK: How Much Excess Heat Is Available from Industrial Sites?". *Sustainability 13(3), 1439. ISSN: 2071-1050. DOI: https://doi.org/10.3390/su13031439*

In this journal paper an approach was developed to investigate industrial excess heat potentials for the EU27+UK. The method applies the developed industry database to assess site-specific potentials from the energy-intensive industries at different temperature levels (25°C, 55°C and 95°C) that can be used for district heating systems. Depending on the temperature level, substantial potential up to nearly 270 TWh/yr could be assessed. The derived industrial excess heat potentials were matched with district heating areas and visualised in GIS.
The data is available on the sEEnergies Open Data Hub https://s-eenergies-open-data-euf.hub.arcgis.com/.

My contribution: Conceptualisation. Co-development and validation of the industry database. Review and editing.

Paper B – Co-author journal publication

Can Industry Keep Gas Distribution Networks Alive? Future Development of the Gas Network in a Decarbonized World: A German Case Study

S. Oberle, M. Neuwirth, T. Gnann and M. Wietschel (2022). "Can Industry Keep Gas Distribution Networks Alive? Future Development of the Gas Network in a Decarbonized World: A German Case Study". *Energies 15(24), 9596. ISSN: 1996-1073. DOI: https://doi.org/10.3390/en15249596*

This analysis aims to identify whether gas distribution networks may have a future role in a decarbonised energy system. The GIS-based comparison of industry sites per sector and their proximity to the gas transport infrastructure shows that around 33% of the energy-intensive industry branches currently rely on natural gas from distribution grids. In addition to households and the residential sector, most industries that are currently supplied by the gas distribution network are likely to undergo electrification of their processes. This projected development indicates an obsolete future role for distribution networks.

My contribution: Conceptualisation. GIS analysis. Explanation of industry characteristics. Evaluation. Review and editing.

Paper C – Co-author conference publication

Deep decarbonisation of the German industry via electricity or gas? A scenario-based comparison of pathways

T. Fleiter, M. Rehfeldt, M. Neuwirth, A. Herbst (2022). "Deep decarbonisation of the German industry via electricity or gas? A scenario-based comparison of pathways". *Eceee Summer Study Proceedings 2020, ISSN: 20017979, 509 - 519, ISBN: 978-919838786-5.* DOI: 10.24406/publica-fhg-409071

In this conference paper, a comparison of two extreme scenario pathways for the German industry is conducted. The first scenario tends towards extreme shares of electricity, wherever electrified processes may be applicable, and the second investigates decarbonisation by using green gases. The results show that most industrial processes can be electrified, while green gases, such as hydrogen, are required for the direct reduction in primary steel production and as feedstocks in the chemical industry.

My contribution: Conceptualisation. Analysis on use of clean gas. Data provisioning. Evaluation. Review and editing.

Paper D – Co-author conference publication

Modelling pathways towards a climate-neutral EU industry sector

K. Al-Dabbas, T.Fleiter, M. Neuwirth, M. Rehfeldt, A. Herbst (2022). "Modelling pathways towards a climate-neutral EU industry sector". *Eceee Summer Study Proceedings 2022, ISSN: 16537025, 1475 - 1483, ISBN: 978-919882700-2.* DOI: 10.24406/publica-212

Many regulations to push industry decarbonisation have been implemented at the EU level in recent years. This conference contribution evaluates different scenario pathways that achieve 95% emission reduction in the industry sector in the EU. Considerable efforts and a fast diffusion of climate-neutral industrial processes, especially for process heat and feedstocks, are necessary to achieve the targets. Electricity demand will increase, and primary steel and basic chemicals production show a robust demand for hydrogen.

My contribution: Conceptualisation. Data provisioning. Evaluation. Review and editing.

Paper E – Co-author conference publication

Pathways to a near carbon-neutral German industry sector by 2045: A model-based scenario comparison and recommendations for action

A. Herbst, T. Fleiter, M. Rehfeldt, M. Neuwirth (2022). "Pathways to a near carbon-neutral German industry sector by 2045: A model-based scenario comparison and recommendations for action". *Eceee Summer Study Proceedings 2022, ISSN: 16537025, 1419 – 1429, ISBN: 978-919882700-2.* DOI: 10.24406/publica-211

Recommendations for action to decarbonise the industry sector require robust results and the need to curtail uncertainties in transition pathways, which are the aim of this conference contribution. Two extreme scenarios are analysed, one representing an electricity-based scenario and the other focussing on hydrogen as a decarbonisation option. For both, technological development and upscaling must be fast to be able to implement technically mature processes, either electrified or hydrogen-based by 2030 and to reach climate goals in 2045.

My contribution: Conceptualisation. Data provisioning. Single analyses. Evaluation. Review and editing.

Presentations

Referring to the contents of this thesis, several presentations were given in front of scientific and industrial audiences:

M. Neuwirth, T. Fleiter, A. Herbst, and M. Rehfeldt: "Potenziale von Wasserstofftechnologien zur Dekarbonisierung der Chemieindustrie in Deutschland"; 16. Symposium Energieinnovation, Graz/Austria; 2020-02-14.
https://www.tugraz.at/events/eninnov2020/nachlese/download-beitraege/stream-b#c279292

M. Neuwirth, T. Fleiter: "Hydrogen technologies for a CO_2-neutral chemical industry - a plant-specific bottom-up assessment of pathways to decarbonise the german chemical industry"; ECEEE Industrial efficiency - Panel 6: Deep decarbonisation of industry, Gothenburg (online); 2020-09-17.
https://www.eceee.org/library/conference_proceedings/eceee_Industrial_Summer_Study/2020/6-deep-decarbonisation-of-industry/hydrogen-technologies-for-a-co2-neutral-chemical-industry-a-plant-specific-bottom-up-assessment-of-pathways-to-decarbonise-the-german-chemical-industry/

M. Neuwirth, M. Khanra, M. Jovicic, M. Shinde, and T. Fleiter: "Future hydrogen demands from industry transition towards 2030 - a site-specific bottom-up assessment for North-Western Europe"; ECEEE 2022 Summer Study - Panel: 9. Deep decarbonisation of industry, Hyères/France; 2022-06-09.
https://www.eceee.org/library/conference_proceedings/eceee_Summer_Studies/2022/9-deep-decarbonisation-of-industry/future-hydrogen-demands-from-industry-transition-towards-2030-a-site-specific-bottom-up-assessment-for-north-western-europe/

M. Neuwirth, Y. Huck, S. Eidelloth, and T. Fleiter: "Anlagenspezifische Modellierung der Transformation in der Europäischen Schwerindustrie"; IEWT 2023 - Industrie II, Vienna/Austria; 2023-02-16.
https://iewt2023.eeg.tuwien.ac.at/download/contribution/presentation/246/246_presentation_20230216_072109.pdf

M. Neuwirth, T. Fleiter: "A plant-specific approach to model future hydrogen demands in energy-intensive industries"; Hydrogen Days 2023, Prague/Czech Republic; 2023-03-31.
https://www.hydrogendays.cz/2023/pages/donwload/index.html

M. Neuwirth, T. Fleiter: "A plant-specific approach to model future hydrogen demands in energy-intensive industries"; Hydrogen Week 2023 - Poster Session, Brussels/Belgium; 2023-11-22.

M. Neuwirth, T. Fleiter: "A plant-specific approach to model future hydrogen demands in energy-intensive industries"; ECEEE Zero Carbon Industry 2024, Antwerp/Belgium; 2024-01-30.
https://www.eceee.org/industry/programme/day-2-january-31/

Scientific reports

As part of the projects I contributed during my PhD time, a selection of scientific project reports is listed following:

T. Fleiter, P. Manz, M. Neuwirth, F. Mildner, U. Persson, K. Kermeli, W. Crijns-Graus, C. Rutten (2020). D5.1. Excess heat potentials of industrial sites in Europe In: sEEnergies Horizon 2020 Project. DOI: `10.24406/publica-fhg-300357`

T. Fleiter, M. Rehfeldt, P. Manz, M. Neuwirth, A. Herbst (2021). Langfristszenarien für die Transformation des Energiesystems in Deutschland 3 - Treibhausgasneutrale Hauptszenarien - Modul Industrie. DOI: `10.24406/publica-fhg-301089`

A. Herbst, T. Fleiter, M. Rehfeldt, M. Neuwirth, U. Fahl, L. Kittel, K. Hufendiek (2021). Industriewende In: G. Luderer, C. Kost, and D. Sörgel (Eds.) (2021): Deutschland auf dem Weg zur Klimaneutralität 2045 - Szenarien und Pfade im Modellvergleich, (Ariadne-Report), Potsdam : Potsdam Institute for Climate Impact Research, 359 p. DOI: `https://doi.org/10.48485/pik.2021.006`

F. Marscheider-Weidemann, S. Langkau, E. Eberling, L. Erdmann, M. Haendel, M. Krail, A. Loibl, C. Neef, M. Neuwirth, L. Rostek,S. Shirinzadeh, D. Stijepic, L.A. Tercero Espinoza, S.-J. Baur, M. Billaud, O. Deubzer, F. Maisel, M. Marwede, J. Rückschloss, and M. Tippner (2022). Raw materials for emerging technologies 2021. ISBN: `ISBN:978-3-948532-62-8`

N. Pieton, M. Neuwirth, M. Jahn, and M. Ragwitz (2022). "Policy Paper zur Sicherstellung einer mittel- bis langfristigen klimaneutralen Rohstoffversorgung der Raffinerie Schwedt". TransHyDE. DOI: `doi:10.24406/publica-478`

M. Wietschel, E. Duetschke, M. Neuwirth et al. (2022). The potential of a hydrogen economy: an economic and social perspective. In: Neugebauer, R. (eds) Hydrogen Technologies. Springer, Cham. DOI: `https://doi.org/10.1007/978-3-031-22100-2_3`

M. Wietschel, F. Roth, J. Fragoso, A. Herbst, C. Kleinschmitt, F. Wittmann, B. Breitschopf, L. Zheng, J. Eckstein, M. Neuwirth et al. (2022). War in Ukraine: Implications for the European and German strategies for importing hydrogen and synthesis products. Position paper DOI: `doi.10.24406/publica-203`

Consentec GmbH, Guidehouse Germany GmbH, Fraunhofer IEG, Fraunhofer ISI, Fraunhofer SCAI, Technische Universität Berlin (E&R) (2023). Systemdienliche Integration von grünem Wasserstoff. `https://www.bmwk.de/Redaktion/DE/Downloads/S-T/studie-systemdienliche-integration-von-gruenem-wasserstoff`

T. Fleiter, M. Rehfeldt, L. Neusel, S. Hirzel, M. Neuwirth, C. Schwotzer, F. Kaiser, C. Gondorf (2024). CO_2-neutral process heat using electrification and hydrogen: Policy Brief. `https://www.isi.fraunhofer.de/content/dam/isi/dokumente/policy-briefs/24-07_policy_brief_process-heat_co2-neutral_%20electrification_hydrogen.pdf`

P. C. Verpoort, F. Ueckerdt, Y. Beck, D. Bietenholz, A. Dertinger, T. Fleiter, A. Grimm, G. Luderer, M. Neuwirth et al. (2024). Transformation der energieintensiven Industrie – Wettbewerbsfähigkeit durch strukturelle Anpassung und grüne Importe. https://ariadneprojekt.de/media/2024/12/Ariadne-Report_GrueneWertschoepfungsketten_Dezember2024.pdf

G. Luderer, F. Bartels, T. Brown, F. Schreyer, D. Sörgel, R. Hasse, J. Hoppe, R. Pietzcker, P. C. Verpoort, T. Gnann, D. Speth, F. Frank, M. Krail, C. Aulich, P. Plötz, H. Nolte, C. Kost, C. Senkpiel, S. Herkel, M. Rehfeldt, A. Herbst, T. Fleiter, M. Neuwirth et al. (2025). Die Energiewende kosteneffizient gestalten – Szenarien zur Klimaneutralität 2045. https://www.isi.fraunhofer.de/content/dam/isi/dokumente/policy-briefs/24-07_policy_brief_process-heat_co2-neutral_%20electrification_hydrogen.pdf

Research projects

Several projects, both national and international, contributed to this thesis or have benefited from the work during this dissertation. The respective project reports are listed in the scientific reports above, where further analyses have been investigated on the data basis of this thesis, or the results could contribute to follow-up questions.

sEEnergies - Quantification of synergies between Energy Efficiency first principle and renewable energy systems; European Commission, Horizon 2020 grant number: 846463.
https://www.seenergies.eu/

VerSEAS - Versorgungssicherheit in einem transformierten Stromsystem mit extremen Anteilen Erneuerbarer Energien und starker Sektorkopplung; BMBF, Grant number: 03EI1018C.
https://www.enargus.de/detail/?id=1419827

TransHyDE-Sys; BMBF - research project; Grant number 03HY201L;
https://www.transhyde.de

TRANSIENCE - TRANSItioning towards an Efficient, carbon-Neutral Circular European industry; European Commission, Horizon Europe grant number: 101137606.
https://www.transience.eu/

RESILIENT - Resilient Energy System Infrastructure Layouts for Industry, E-Fuels and Network Transitions; CETPartnership project: Grant number: 03EI4083B;
https://resilient-project.github.io/

Langfristszenarien III - für die Transformation des Energiesystems in Deutschland; BMWK; Grant number: 03MAP392.
https://langfristszenarien.de/

Ariadne; BMBF - research project; Grant number: 03SFK5D0.
https://ariadneprojekt.de/

Ariadne 2; BMBF - research project; Grant number 03SFK5D0-2.
https://ariadneprojekt.de/

H2-Lieferkette Nordwesteuropa; BMBF; Grant number: 01DS23012.

H2-Masterplan Ostdeutschland; VNG;
https://h2-masterplan-ost.de/

H2-Systemintegration - Systemdienliche Integration von grünem Wasserstoff; BMWK; Grant number: 03MAP405
https://www.bmwk.de/Redaktion/DE/Downloads/S-T/studie-systemdienliche-integration-von-gruenem-wasserstoff.pdf

Poster

Parts of this work were exposed in poster format at:

European Hydrogen Week; Brussels, 2023

TransHyDE plenary meeting; Leipzig, 2024

TransHyDE final event; Berlin, 2025

About the author

Lindau/Bodensee in southern Germany is the place where Marius Neuwirth was born in 1994 and passed his final exams (Abitur) in 2013.
For his studies in Chemical and Process Engineering, he moved to Karlsruhe and graduated with a Master's degree at the Karlsruhe Institute of Technology (KIT) in 2019. During his Master thesis, he visited the TU Wien for a collaboration.
In 2019 he started a research position at Fraunhofer Institute for Systems- and Innovation Research (ISI) in the Competence Center for Energy Systems and Energy Technology. He registered for a PhD at the Institute of Energy Systems and Thermodynamics at TU Wien in 2021. During his scientific work, contributions to several research projects, such as *"sEEnergies"*, *"TRANSIENCE"*, *"TransHyDE-Sys"*, *"RESILIENT"*, *"VerSEAS"*, *"Ariadne"*, and others formed the basis for the present dissertation.

A complete list of the author's publications can be found at https://publica.fraunhofer.de and all peer-reviewed scientific articles are updated on and https://orcid.org/0000-0002-1975-8626.