Integration Potentials of Electrolytic Hydrogen and Synthetic Fuels into the German Energy System: A Socio-Techno-Economic Analysis

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Zusammenfassung

Elektrolyse-Wasserstoff und strombasierten, synthetischen Kraftstoffen wird im Kontext der Energiewende eine Schlüsselrolle zugesprochen, um anteilig die Volatilität der erneuerbaren Stromerzeugung zu kompensieren und energieintensive Anwendungen außerhalb des Stromsektors mit erneuerbarer Energie zu versorgen. Möglichkeiten der Integration dieser auf Basis so genannter Power-to-Fuel Konzepte hergestellten erneuerbaren Energieträger in das Energiesystem unterliegen indes komplexen soziotechnischen und sozioökonomischen Zusammenhängen. Bis heute sind ausschließlich geförderte Pilotprojekte realisiert, da Geschäftsmodelle für die Produktion von Elektrolyse-Wasserstoff und strombasierten, synthetischen Kohlenwasserstoffen aller Art, wenn überhaupt, bislang nur in kleinen Nischenmärkten wirtschaftlich umzusetzen sind. Darüber hinaus gibt es bisher kaum Erfahrungswerte, wie flexibel entsprechende Anlagen auf ein fluktuierendes Stromangebot reagieren und dadurch Stromnetze entlasten können.

Die vorliegende Dissertation setzt an diesem Status quo an und adressiert drei übergeordnete Fragestellungen: (1) Wie kann eine wirtschaftliche Integration von Power-to-Fuel Konzepten in Deutschland gelingen und unter welchen Bedingungen können erfolgreiche Geschäftsmodelle für den Betrieb der Anlagen entstehen? (2) Können Power-to-Fuel Konzepte so flexibel betrieben und so großskalig aufgebaut werden, dass Stromnetze entlastet und weite Teile nicht direkt elektrifizierbarer Anwendungen in den Sektoren Verkehr und Industrie mit Kraft- und Brennstoffen sowie Basischemikalien versorgt werden können? (3) Resultiert aus einer Integration von Power-to-Fuel Konzepten in Deutschland eine übermäßige finanzielle Belastung für private Haushalte und kommerzielle Verbraucher?

Im Rahmen von vier Publikationen werden die drei Fragestellungen auf Basis ausgewählter Methoden wie unter anderem der Anwendung innovationstheoretischer Modelle, der agentenbasierten Modellierung und der Prozesssimulation adressiert und Erkenntnisse für eine erfolgreiche Integration erlangt. Die Ergebnisse zeigen deutlich auf, dass eine großskalige Integration in Deutschland und damit verbundene Treibhausgaseinsparungen auf volkswirtschaftlicher Ebene durch vermiedene Umweltfolgekosten deutliche Kostenvorteile gegenüber einer weitgehend auf fossilen Energieträgern basierenden Energieversorgung bietet. Auf betriebswirtschaftlicher Ebene ergeben sich bislang jedoch kaum Spielräume für die Entstehung von Geschäftsmodellen. Für eine umfängliche Integration in Deutschland sind daher umfangreiche Änderungen energiepolitischer Rahmenbedingungen erforderlich, um einen zügigen Markthochlauf zu initiieren. Ergebnisse der agentenbasierten Modellierung zeigen, dass insbesondere eine kurzfristige, sehr hohe Förderung von Power-to-Fuel Anlagen hohe private Investitionen auslöst, welche zu einer frühzeitigen Kostensenkung der Technologien führen können. Zusätzlich trägt eine Verschärfung und Ausweitung von

Quoten zur Treibhausgasminderung für Unternehmen zur Steigerung der Nachfrage nach Elektrolyse-Wasserstoff und strombasierten, synthetischen Kraftstoffen bei. Demgegenüber rufen auch die kürzlich sehr stark gestiegenen Preise für konventionelle Energieträger noch keine unmittelbare Konkurrenzfähigkeit von Power-to-Fuel Produkten hervor. Ein flexibler Betrieb von Power-to-Fuel Anlagen in Abhängigkeit des erneuerbaren Stromangebotes ist grundsätzlich möglich, im Prozessschritt der Kohlenwasserstoffsynthese jedoch deutlich eingeschränkt. Die Niedertemperatur Wasser-Elektrolyse bietet indes ein in hohes Maß an Flexibilität und ermöglicht stromangebotsorientierte Betriebsstrategien. Im Vergleich zu Energiepreisentwicklungen in den vergangenen Jahrzehnten können etwaige kurz- bis mittelfristige Preissteigerungen für Verbraucher durch eine sukzessive Einführung von Elektrolyse-Wasserstoff und strombasierten, synthetischen Kraftstoffen als moderat eingestuft werden, während in der Langzeitperspektive Elektrolyse-Wasserstoff voraussichtlich deutlich kostengünstiger als konventionelle Energieträger verfügbar sein wird.

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Abstract

Electrolytic hydrogen and electricity-based synthetic fuels are considered crucial for a holistic energy system transition to compensate for the volatility of renewable electricity generation and to supply energy-intensive applications in other sectors with renewable energy. A successful integration of these renewable energy carriers, produced via so-called Power-to-Fuel concepts, is subject to complex socio-technical and socio-economic constraints. To date, only funded pilot projects have been realized since successful business models for producing electrolytic hydrogen and electricity-based synthetic hydrocarbons of all kinds can only be implemented economically in small niche markets, if at all. In addition, there is hardly any empirical data on how flexible plants can react to a fluctuating electricity supply and relieve electricity grids by this means.

Based on this status quo as a starting point, three central research questions are addressed in this dissertation: (1) How can an economical implementation of Power-to-Fuel concepts be achieved in Germany, and which conditions allow for the development of business models? (2) Are Power-to-Fuel concepts suitable for dynamic operation modes, and is upscaling to large capacities possible for the provision of sufficient fuel quantities for the industry and mobility sector? (3) Does an integration of Power-to-Fuel concepts in Germany result in an excessive financial burden for private households and commercial consumers?

Within the framework of four publications, the three questions are addressed based on selected methods such as the application of innovation theory-based models, agent-based modeling, and process simulation, among others. The results clearly show that a large-scale integration in Germany and the associated greenhouse gas savings offer significant cost advantages at the macroeconomic level through avoided environmental impact costs compared to an ongoing energy supply, which is primarily based on fossil fuels. At the business level, however, there has so far been little scope for the emergence of business models. For a large-scale integration in Germany, extensive changes in energy policy framework conditions are required to initiate a rapid market rollout. Agent-based modeling results show that especially a very high short-term subsidization of Power-to-Fuel plants can trigger high private investments, which can lead to an early cost reduction of the technologies. Furthermore, an expansion of greenhouse gas reduction quotas for companies contributes to increased demand for electrolytic hydrogen and electricity-based synthetic fuels. In contrast, even the recent very sharp increase in prices for conventional energy sources does not yet evoke the immediate competitiveness of Power-to-Fuel products. Flexible operation of Power-to-Fuel plants according to renewable power supply patterns is generally possible, but significantly limited in the hydrocarbon synthesis process step. Low-temperature water electrolysis, however, offers a high degree of flexibility and enables electricity supply-oriented operation strategies. Compared to energy price developments in the past decades, any short- to medium-term price increases for consumers as a consequence of a successive introduction of electrolytic hydrogen and electricity-based synthetic fuels can be considered moderate. Moreover, in the long-term perspective, electrolytic hydrogen is expected to be available at significantly lower prices than conventional energy sources.

Highlights

- A qualitative innovation theory-based model is transformed into a simulation tool, enabling quantifiable insights into Power-to-Fuel market integration strategies and potentials.
- A quasi-dynamic electrolysis model for alkaline and proton exchange membrane electrolysis technologies is developed to gain an in-depth understanding of the limitations of dynamic operation modes.
- An advanced techno-economic analysis approach enables a cost-optimized electrolysis capacity design according to renewable electricity supply profiles.
- Agent-based modeling results provide policy recommendations for a successful and sustainable PtF integration into the German energy markets and reflect that rather a set of regulatory adjustments is required instead of merely single modifications.
- A socio-economic analysis shows significant benefits for a PtF integration compared to an ongoing fossil fuel supply in terms of national energy-related expenses.
- Considerations of current geopolitical tensions underpin that an early PtF integration is also beneficial from an economic point of view.

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List of Publications

C. Schnuelle, J. Thoeming, T. Wassermann, P. Thier, A. von Gleich (2019): Socio-technical-economic assessment of power-to-X: Potentials and limitations for an integration into the German energy system, *Energy Research & Social Science 51*, 187-197, https://doi.org/10.1016/j.erss.2019.01.017

C. Schnuelle, T. Wassermann, D. Fuhrlaender, E. Zondervan (2020): Dynamic hydrogen production from PV & wind direct electricity supply - Modeling and techno-economic assessment, *International Journal of Hydrogen Energy 45*, 29938-29952, https://doi.org/10.1016/j.ijhydene.2020.08.044

C. Schnuelle, K. Kisjes, T. Stuehrmann, P. Thier, I. Nikolic, A. von Gleich, S. Goessling-Reisemann (2020): From Niche to Market - An Agent-Based Modeling Approach for the Economic Uptake of Electro-Fuels (Power-to-Fuel) in the German Energy System, *Energies 13*, No. 522, https://doi.org/10.3390/en13205522

C. Schnuelle, T. Wassermann, T. Stuehrmann (2022): Mind the Gap - A Socio-Economic Debate on Price Developments of Green Hydrogen, Synthetic Fuels and Conventional Energy Carriers in Germany, *Energies 15*, No. 3541, https://doi.org/10.3390/en15103541

Accompanying Publications

C. Schnuelle, P. Kenkel, T. Wassermann (2020): Multikriterielle Bewertung von Elektrolyse- und CO_2-Capture Technologien für eine Power-to-Methanol Prozesskette, *artec paper*, Nr. 223, ISSN: 1613-4907

C. Schnuelle, T. Wassermann, M. Kalis, J. Schäfer (2021): Ausgewählte Standortfaktoren für Power-to-Fuel Anlagen: Erdölraffinerie versus grüne Wiese, *Energiewirtschaftliche Tagesfragen 71*, Heft 7-8

Contents

List of Abbreviations

ABM	Agent-based modeling
ACAPEX	Annualized capital expenditures
AEL	Alkaline electrolysis
AEMEL	Anion exchange membrane electrolysis
AHP	Analytical Hierarchy Process
CAPEX	Capital expenditures
CRTL	Control
CCU	Carbon Capture and Utilization
DAC	Direct air capture
DC	Direct current
DRI	Direct reduced iron
EEG	Erneuerbare-Energien-Gesetz
ELY	Electrolyte pumping
ETS	Emissions Trading System
FCI	Fixed capital investment
FT	Fischer-Tropsch synthesis
GHG	Greenhouse gas
HP	High-pressure
HT	High-temperature
HTFT	High-temperature Fischer-Tropsch synthesis
KOH	Potassium hydroxide lye
KPIs	Key performance indicators
LHV	Lower heating value
LP	Low-pressure
LT	Low-temperature
LTFT	Low-temperature Fischer-Tropsch synthesis
MCDA	Multi-criteria decision analysis
MEA	Monoethanolamine
MLP	Multi-Level-Perspective
NaOH	Sodium hydroxide lye
NPC	Net production costs
OPEX	Operational expenditures

PC	Purchased cost of equipment
PEM	Proton exchange membrane
PEMEL	Proton exchange membrane electrolysis
PMP	Pump
PWR	Power
PtF	Power-to-Fuel
PtX	Power-to-X
PV	Photovoltaic
R&D	Research and development
RE	Renewable energy
RF	Ratio factor
RWGS	Reverse water-gas shift reaction
SDGs	Sustainable Development Goals
SOEL	Solid oxide electrolysis
TEA	Techno-economic analyses
TRL	Technology Readiness Level
TSA	Temperature swing adsorption
WSM	Weighted Sum Model

Chapter I

1. Introduction

1.1. Motivation and Objective

Within the 1992 United Nations Conference on Environment and Development (UNCED) in Rio de Janeiro, Brazil, more than 178 countries adopted the so-called Agenda 21 – an action plan to initiate a global partnership for sustainable development to improve human lives and protect the environment [1]. In September 2015, a shared call for action was adopted by all United Nations member states with the outcome of the prominent *17 Sustainable Development Goals* (SDGs) [2]. The global threat of climate change and its mitigation is directly addressed by SDG 13 and indirectly supported by others, of which especially SDG 7 'Affordable and Clean Energy' is to be mentioned. A few months later, 196 countries agreed to the so-called *Paris Agreement* at the United Nations Climate Change Conference (COP21) in December 2015, a legally binding treaty to limit global warming to well below 2 °C, preferably to 1.5 °C, compared to pre-industrial levels [3]. The rapid mitigation of anthropogenic greenhouse gas (GHG) emissions, which are primarily related to our energy systems, is key to achieving this target.

In Germany, the national energy system transition (*Energiewende*) achieved considerable progress as the net electricity production from renewable energy (RE) sources already reached a share of 50.3 % in 2020 [4]. However, debates and efforts were mainly focused on the electricity sector, whereas GHG mitigation in other energy-intensive sectors like heat and industry remains rather unsatisfactory [5]. In contrast, the 2019 GHG emissions of the transport sector reached an even higher value compared to the 1990 reference, followed by a declining trend in 2020 and 2021, which is mainly correlated to the COVID-19 pandemic effects [6]. The renewable share in the transport sector is primarily provided in the form of biofuels so far, whose maximum production potential is considered below 500 TWh a^{-1} in Germany due to the scarcity of appropriate farming land and low energy yield per unit area [7–9].

With a considerably higher achievable area-specific energy yield via photovoltaic and wind power, renewable electricity is expected to serve as the primary energy source in future energy systems. Due to the volatile nature of solar and wind energy, however, large capacities of photovoltaic and wind power installations with relatively low full-load hours will be required beside strategies to bridge temporal gaps between supply and demand patterns [10]. In this context, the *Energiewende* is supposed to have reached a new transition phase – represented by the term *sector coupling* renewable electricity shall be provided to all other energy sectors [11].

Direct electrification of all energy-intense applications, nonetheless, is rather critical, if not even impossible. This applies especially for technical processes where energy carriers serve as reducing agents as well as for applications that require a high volumetric energy density, such as aviation and road- or sea-bound heavy-duty transport [12].

The concepts of so-called *Power-to-Fuel* (PtF) processes are promising technology paths for both, balancing volatile electricity production patterns as well as providing energy carriers with high energy density to all sectors [13,14]. In these concepts, water electrolysis is applied for the production of hydrogen, which is crucial for all further steps along PtF process chains. Thus, water electrolysis can be considered a key technology for future energy systems, with hydrogen being applied directly as an energy carrier, reactant, or feedstock for producing hydrocarbon fuels and platform chemicals, e.g. methanol or ethylene [15,16]. For the latter ones, CO_2 (or CO) and hydrogen are typically synthesized into liquid and gaseous hydrocarbons via methanation, Fischer-Tropsch, or methanol synthesis process routes [17]. Ambient air and point sources such as (industrial) combustion processes can serve as typical sources for carbon capture and utilization (CCU) processes, which can be realized via absorption, adsorption, and membrane technologies, among others [18,19]. Depending on the synthesis path and subsequent upgrading processes, synthetic fuels such as methane, methanol, and crude oil with the typical fractions of petrol, diesel, and jet fuel can be generated and substitute conventional counterparts one-to-one [20]. Hence, PtF concepts represent hydrogen production via water electrolysis as well as rather complex process chains for synthetic fuel production, which can be designed in a large variety of technology combinations [21]. Independent of the final product, a rigorous contribution to greenhouse gas mitigation can be achieved. In this regard, a renewable electricity source for water electrolysis is crucial, among other aspects [22].

According to the technological benefits, PtF concepts may contribute to solve central problems of the energy system transition process, as they can provide *indirect electrification* within all sectors besides a relief of electricity grids in the form of supply-orientated operation modes [23]. In this context, many studies see PtF concepts as an essential part of future energy systems, and in the meantime, implementation strategies also became part of political agendas, e.g. the announced German water electrolysis capacity target of 10 GW_{el} until 2030 with a production volume of 14 TWh, respectively [24]. Not only in Germany but worldwide, huge funding volumes are available or in preparation to promote the implementation of hydrogen and synthetic fuels [25,26].

To date, PtF plants have been successfully operated within demonstration projects, as more than 30 pilot plants with an accumulated electrolysis capacity above 25 MW_{el} have yet been realized [27]. However, a large-scale implementation of these technologies beyond funded pilot projects is still to be developed.

Although several prominent scenarios expect an annual future electrolytic hydrogen and synthetic fuel demand of up to 800 TWh in Germany, specific strategies for a rapid realization of huge PtF capacities are missing [28]. Due to high investment as well as operational costs, the concept is rather unattractive from an economic point of view by now. Consequently, the question of how to implement PtF concepts within the established energy markets remains widely open. Whereas current production costs of electrolytic hydrogen differ according to a literature review (cf. Chapter IX) in a huge range between 9.9-18.9 ct kWh^{-1}, synthetic liquid fuels come at even higher production costs of 38.7-49.7 ct kWh^{-1} [29]. Both price levels clearly exceeded typical prices for conventional natural gas and crude oil-based products within recent years. However, the latter ones drastically increased in price lately due to current geopolitical tensions. As such, natural gas reached spot market prices above 20 ct kWh^{-1} in March 2022, petrol prices peaked above 11 ct kWh^{-1} [30]. Accordingly, the price gap between conventional fuels and renewable substitutes shrank or partly vanished. Even though this circumstance may be beneficial for the economic competitiveness of renewable fuels, the youngest price levels cause critical global constraints and provoke new socio-economic difficulties.

From a technical point of view, rather limited knowledge on intermittent operation modes of specific technologies along the PtF process chain is available in the literature. Whereas one beneficial aspect of PtF concepts is a general ability for dynamic responses to fluctuating renewable electricity supplies, detailed information on technical constraints and consequential effects such as material degradation is lacking so far. In addition, the availability of critical materials, e.g. iridium for fuel cells or proton exchange membrane electrolysis cells, needs to be taken under consideration in the context of a large-scale implementation of these technologies.

Thus, despite the demonstration of PtF concepts in pilot plants, important research questions are still widely open with respect to a successful large-scale energy system integration. Due to the intersectoral applicability and the vast spectrum of involved interdisciplinary stakeholders, PtF concepts can be interpreted as so-called *system innovations*[1], which interfere with an immense variety of impact factors, e.g. political regulation and promotion, technology development, customer demand and societal desires (cf. Chapter VIII). To cover all aspects of these complex interrelations, this work applies curated socio-techno-economic analysis approaches and addresses the following three research questions at its heart:

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[1] System innovation: According to Fischedick et al. system innovations can only deploy their technical functionality within complex and dynamic systems, if they are supported by incorporated social and infrastructural innovation elements [11].

1. What are expectable technical limitations of PtF concepts according to dynamic operation strategies and scarce material deployment?
2. How can PtF concepts be successfully integrated into the German energy markets?
3. To which extent may PtF concepts provoke or attenuate financial burdens for households and enterprises in Germany?

These research questions are motivated by the initial hypothesis that a successful energy system transition towards 100 % renewable energies in all energy-intensive sectors is impossible without PtF concepts. The following subchapter provides a brief overview of how and in which chapters these research questions are addressed in detail.

1.2 On the Structure of this Thesis

The above-described objective is covered in six compiled publications, of which four represent a central element of this dissertation. Within Chapter II–Chapter V, relevant background information and the methodological approaches are described before the major results and further research requirements are briefly discussed and concluded. Chapter I–Chapter V are consequently designed as a comprehensive summary of all relevant contents of this dissertation, before detailed information on the individual working tasks is subsequently provided within the publications in Chapter VI–Chapter IX and within the Appendix.

The first research question is addressed in two publications. In Chapter VI, limitations for a large-scale integration of PtF concepts in Germany are discussed predominantly qualitatively from a system-level perspective, especially focusing on dynamic plant operability, material scarcity, social acceptance, and economic relations. Chapter VII follows up on the subject of dynamic plant operation modes and focuses on a quantitative investigation of technical potentials and consequential techno-economic key performance indicators (KPIs). The analysis is based on a compiled simulation tool for low-temperature electrolysis technologies, enabling the modeling of specific operating characteristics in relation to photovoltaic (PV) and wind power generation patterns. The insights are further applied for a detailed techno-economic assessment of selected operation strategies and consequential hydrogen production costs.

The topic of how to implement PtF concepts into the German energy markets is addressed in Chapter VIII. Here, an agent-based modeling approach is applied to quantitatively investigate the key parameters, enabling applicable business models for PtF plants. The underlying simulation tool is orientated to and backed by specific energy system-related innovation theories. In this context, impacts of interdisciplinary aspects from the fields of policy, regulation, societal acceptance, technological innovation, stakeholder behavior, and economics are analyzed with regard to the development of PtF capacities in Germany until 2035. Whereas Chapter VI–Chapter VIII investigate the potentials and limitations for a successful PtF integration in Germany, the socio-economic consequences of a broad diffusion of these technologies are discussed in Chapter IX. The topic is addressed under the given circumstance that synthetic fuels will, at least in the short- and medium-term, only be available at considerably higher prices compared to those of conventional counterparts until the recent past (before the massive energy price increases in consequence of the Ukraine war). Based on literature data, projected price developments until 2050 are discussed and correlated to former price dynamics back till the 1950s. Subsequently, a conclusion on whether customers face an increased financial burden from a successful large-scale implementation into the German energy system is developed.

Chapter II

2. Background and State of the Art of Power-to-Fuel Concepts

Large-scale electrolytic hydrogen production via alkaline electrolysis is already established for decades. A prominent plant has been operated in Aswan, Egypt, since 1963 with an initially installed capacity of 203 MW_{el} [31]. However, modern plant designs of electrolyzers for PtF concepts are rather different from former installations (cf. Section 2.2.1). Also, synthetic fuel production via Fischer-Tropsch Synthesis is a very mature technology already developed and in operation since the 1920s [32]. Large capacities for the production of synthetic fuels exist worldwide, e.g. liquid fuel production based on syngas in Pearl, Qatar [33]. The idea of a renewable electricity-based synthetic fuel production in the context of energy system transitions is rather young instead. The first German literature information, as well as the first German project for synthetic methane production, is dated to 2008. The so-called *Power-to-Gas* concept was introduced by the ZSW (Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg), which realized a 25 kW_{el} demonstration plant including water electrolysis, CO_2 capture from ambient air and a chemical fixed bed reactor for methanation in 2009 [14]. During the last decade, many research projects proved and optimized the production of electrolytic hydrogen as well as synthetic fuels. To date, the worldwide largest PtF plant is operated in Germany within the REFHYNE project in Wesseling with an installed electrolysis capacity of 10 MW_{el} [34]. With the large variety of projects and related research articles, many different terms developed for the underlying process concepts and products, such as Power-to-Gas, Power-to-Hydrogen, Power-to-Liquid, Power-to-X, efuels, powerfuels, and synfuels, among others.

In this work, the concept is generally termed Power-to-Fuel (PtF), independent from the final product. Moreover, the final products are classified as either PtF products or separately as electrolytic hydrogen and synthetic fuels. The following subchapters will provide an executive overview and background information on PtF concepts in the context of the German energy system (Subchapter 2.1) and technical fundamentals and KPIs of the major technologies along PtF process chains (Subchapter 2.2).

1.1 Potentials and Limitations for Power-to-Fuel in Germany

Indirect electrification via electrolytic hydrogen and synthetic fuels is considered as the backbone for the energy transition process in terms of sector coupling, besides *direct electrification* approaches. Although a broad agreement exists among experts about the requirement of both electrification types, expectations on future demand deviate significantly. This is mainly correlated to different assumptions and stakeholder interests regarding suitable applications for PtF products. From an energetic point of view, these renewable fuels should only be applied for industrial processes and transport applications that are not available for *direct electrification* options [35]. Thus, especially within the heating sector and individual traffic concepts, *direct electrification* approaches should be realized as a first choice due to higher efficiency and sufficiency [22,36]. In contrast, another position in this debate is a much broader application of electrolytic hydrogen and synthetic fuels due to the compatibility with existing infrastructures, frugal storage capabilities, a wide range of possible applications, and high acceptance in public, among others.

In Chapter VI and Chapter VIII, three scenarios from 2014 and 2015 on future demand for electrolytic hydrogen and synthetic fuels are discussed in the context of implementation strategies investigation (cf. [37–39]). While all of the scenarios are in accord with ambitious climate protection targets, the bandwidth of assumed PtF capacities and corresponding fuel demand is somewhat differing. Ueckerdt et al. compiled recent scenarios developed in 2021, reflecting the above-discussed diverging perspectives on suitable applications for electrolytic hydrogen and synthetic fuels [28]. Figure 2.1 displays capacity and fuel demand bandwidths according to the scenarios discussed in Chapter VIII and those reflected by Ueckerdt et al. until 2050.

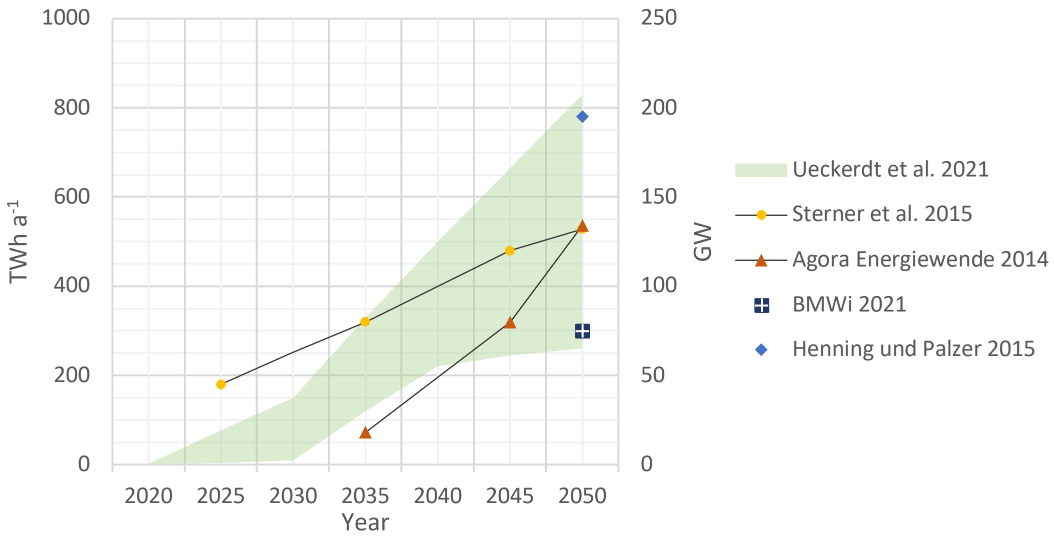

Figure 2.1: Comparison of chosen scenarios for future PtF product demand and installed capacities in Germany. The PtF product demand bandwidth (green) displays data from a variety of topical scenarios based on Ueckerdt et al. [28]. Values of Sterner et al., Agora Energiewende, BMWi, and Henning and Palzer show prospected national PtF capacity demand in Germany [10,38–40]. The BMWi 2021 value for 2050 represents the upper range of the BMWi TN scenarios.

A potential PtF product demand between 10-150 TWh in 2030 can be derived from Figure 2.1, showing that the announced hydrogen target of 14 TWh_{H2} in the coalition treaty of the German government is positioned at the lower demand range. In 2050 PtF product demand will increase to 260-840 TWh.

The electrolytic hydrogen and synthetic fuel production potential in Germany is directly linked to the expansion of wind and PV power plants in Germany and thus to the general availability of renewable electricity. On the other hand, it is also strongly dependent on assumptions about Germany's overall future electricity demand. In a prominent study by Quaschning et al., the future German electricity demand resulting from a successful energy system transition is calculated between 1,320–3,120 TWh a^{-1} and includes electricity supply for PtF processes [41], while the technical potential for PV and wind farms is considered 900 TWh a^{-1} with a respective capacity of 225 GW in a study by Sterner and Specht [14]. Hence, despite a broad diffusion of RE and PtF capacities in Germany, a remaining supply-demand gap will need to be closed via additional imports from abroad.

1.2 Power-to-Fuel Technologies

In the following sections, crucial technologies for PtF concepts are briefly characterized. They are categorized into water electrolysis, CO_2 capture, hydrocarbon synthesis, and product upgrading. For detailed information on the overall idea of PtF concepts, the large variety of possible process chain configurations and applications, as well as technical details it is referred to Dieterich et al. and Breuer et al. [16,17], whereas a comprehensive overview of the development of the concepts from the early beginnings in the 2000s until the recent past is given by M. Sterner and M. Specht 2021 [14].

2.2.1 Electrolysis

The electrochemical splitting of water into hydrogen and oxygen is considered the first step of the process chain and crucial for all PtF concepts. To date, four promising electrolysis technologies are available at a technology readiness level (TRL) of 5 or better, meaning that operation beyond laboratory scale is generally proven. This applies to low-temperature (LT) technologies of alkaline electrolysis (AEL) (TRL 9), proton exchange membrane electrolysis (PEMEL) (TRL 8-9), and anion exchange membrane electrolysis (AEMEL) (TRL 5), as well as to the high-temperature (HT) technology of solid oxide electrolysis (SOEL) (TRL 6-7) [42–45]. KPIs of these technologies are provided in Table 2.1. Other promising concepts are the so-called high-frequency electrolysis, saltwater-co-electrolysis as well as the recently published capillary electrolysis design [46–48]. However, the latter ones are not commercially available yet.

Basically, two electrodes, a semipermeable membrane, and an electrolyte are required beside water as starting material and electrical energy to activate the endothermic redox reaction and corresponding hydrogen production at the cathode side and oxygen production at the anode side [49]. Whereas the underlying electricity demand strongly depends on the specific electrolysis technology, water demand can be considered equal for all LT technologies. In theory, eight liters of water are required to yield 1 kg_{H2} or 33.33 kWh_{H2}, respectively. Due to losses, e.g. by water purification, actual water demand is considerably higher at 15 l kg_{H2}^{-1} for LT technologies and 9.1 l kg_{H2}^{-1} for HT electrolysis [50,51].

The basic design of alkaline electrolysis systems is usually identical for all plants and consists of several subsystems. The specific cell design improved over time from a conventional assembly with a defined distance between the electrodes to the so-called zero-gap assembly, where electrodes are pressed directly onto the separator to reduce ohmic losses. The subsystems can be categorized into electrolysis stacks, thermo- and fluid management, system control, power electronics, plant periphery, and product gas purification [52].

Within the electrolysis stack, cathode and anode are connected to a direct current (DC) source. Both electrodes typically consist of perforated metal sheets and are located close to a diaphragm, a current permeable separator usually based on yttria-doped zirconia or sulfonated polyetheretherketone [53]. The resulting half cells contain a liquid electrolyte such as aquatic potassium hydroxide lye (KOH) or sodium hydroxide lye (NaOH). The electrolyte is pumped through the stack, where the product gases are formed [54]. Phase separation of liquid electrolyte and product gases is mainly realized in large separate tanks with high retention time. Drying and purification are the next logical steps before compression to desired pressure levels [49]. For further information on the electrochemical reactions and thermodynamic interrelations, it is referred to Chapter VII, where cell characteristics and overall plant details are described comprehensively in the context of electrolysis simulation and modeling.

Electrical efficiency of single stacks is stated between 63-71 % at full load and up to 83 % at part load operation related to the lower heating value (LHV) of hydrogen, whereas the overall plant efficiency achieves 51-60 %. Typical plant lifetime is expected between 55,000-120,000 h, depending on operation patterns [49,55].

While alkaline electrolyzers are commercially available at lower capital costs compared to other electrolysis technologies, a significant drawback of this technology, as frequently reported, is its limited operational flexibility with comparatively small part-load ranges, long start-up times, and slow load changes. Information on cold-start behavior deviates drastically in literature and is specified as high as up to two hours. Nevertheless, the AEL technology achieved significant improvements on these issues in recent years, enabling a technical qualification for the provision of primary control reserve [56,57]. The typically applied nickel catalysts are rather vulnerable and tend to a faster degradation rate at dynamic operation modes. However, maintenance costs of only 2-3 % a^{-1} are defined in the literature [49]. Detailed consideration of maintenance and stack replacement costs in relation to dynamic operation strategies is provided in Chapter VII within a dynamic techno-economic analysis approach.

Stacks of PEM electrolyzers generally follow equal design concepts, independent of the technology provider. The cells consist of two electrodes separated through a Nafion-based solid proton exchange membrane, which performs as the electrolyte, catalyst carrier, and separator for product gases. This setup is called membrane electrode assembly (MEA). The main benefits of this technology are the comparably compact cell designs that allow a small footprint, the renunciation of a liquid electrolyte circuit, which reduces plant complexity, as well as a possible operation at high (differential) pressures, so that subsequent compression is not necessarily required. Another benefit compared to the AEL technology is its higher current density which allows for a smaller footprint [43,56].

In contrast to the AEL technology, water is provided to the anode side and decomposed into hydrogen ions and oxygen, leading to a stoichiometric composition of two electrons, two protons, and a half oxygen molecule (cf. Table 2.1).

Further research and development (R&D) requirement is particularly seen in the field of noble metal substitution or reduction. Especially platinum, ruthenium, and iridium supplies can be considered potentially critical as worldwide demand is expected to increase drastically (cf. Chapter VI) [58]. In addition, capital and maintenance costs clearly exceed those of AEL electrolysis systems. Stack efficiencies of 60-68 % can be achieved related to the LHV, while 46-60 % are reported for the system level. A load range of 5-200 % (according to nominal load) significantly outperforms the AEL technology. The same applies to the cold-start availability, which requires only a few seconds [49]. Detailed insights on the comparison of AEL and PEMEL technology concerning the dynamic operation and techno-economic consequences are provided in Chapter VII.

AEMEL electrolysis is still a developing technology and has been commercialized by only one technology provider in small-scale systems yet [42]. The technological concept differs from AEL as the conventional diaphragm is replaced by an anion exchange membrane, allowing the utilization of distilled water or low concentrated alkaline solutions instead of concentrated and corrosive KOH lye. Compared to PEMEL, it replaces the highly acidic and expensive Nafion-based membrane and thus enables the utilization of low-cost transition metals instead of noble metals as a catalyst. In addition, high power densities and a compact plant design are possible. Hence, AEMEL technology combines the advantages of AEL and PEMEL, but suffers from poor long-term stability yet [59,60].

The development of SOEL systems began in the 1970s and gained increasing attention in recent years. The significantly higher temperature level of 700-900 °C and a utilization of water vapor enable electrical efficiencies of up to 100 %. This results from favorable thermodynamics and faster kinetics at high operating temperatures [61,62]. The high-temperature level, however, is challenging according to the long-term stability of plant components. Components of the underlying ceramic electrolyte feature different thermal expansion coefficients, causing potential damage to contacts between electrodes and electrolyte and thus higher cell resistances [53]. Compared to the AEL and PEMEL technologies, SOEL is not yet rated as an industrially mature technology. As such, systems as well as individual stack configurations differ drastically from case to case and are rather tailored to the particular application requirements. In addition, the applied source of high-temperature heat requires a specific thermo- and fluid management design [52].

Water vapor is fed at the cathode side and reduced to hydrogen and oxygen ions (O_{2-}). The reactive oxygen ions pass the ceramic membrane to the anode side and anodize to oxygen. Although only comparatively small pilot plants have been realized so far, large-scale applications are in the planning for the near future. Further R&D demand is correlated to an improvement of cell mechanics as well as a reduction of critical element demand [52]. The latter involves primarily yttrium, lanthanum, strontium, and cobalt [63].

A steep capital cost reduction of currently above 2,000 € kW^{-1} is expected when a series production of the SOEL technology is achieved. Maintenance costs are rated significantly higher compared to LT technologies. This corresponds with a low plant lifetime of 8,000-20,000 h and high degradation rates of 3-50 % a^{-1} [49].

Table 2.1: Overview of techno-economic key performance indicators of selected low-temperature electrolysis technologies. Data is based on Buttler and Spliethoff, Smolinka et al., Holst et al., and IRENA [49,52,59,64].

Category	**Unit**	**AEL**	**PEMEL**	**SOEL**	**AEMEL**
TRL	-	9	8-9	6-7	5
Technology provider examples	-	McPhy, ThyssenKrupp, NEL Hydrogen, ELB	Siemens Energy, ITM Power, ArevaH2Gen, Hydrogenics	Sunfire, Haldor Topsoe	Enapter
Electricity demand stack	kWh Nm^{-3}	4.2-4.8	4.4-5.0	3-3.5	4.8-6.9
Electricity demand system	kWh Nm^{-3}	5.0-5.9	5.0-6.5	3.7-3.9	-
Load flexibility	% of nom. load	25-150	0-200	30-120	3-105
Ramp speed	%P s^{-1}	33	10-100	-	-
Stack lifetime	h	55,000-120,000	60,000-100,000	8,000-20,000	5,000-35,000
Degradation rate	% a^{-1}	0.2-1.5	0.5-2.5	3-50	-
Current density	A cm^{-2}	0.25-0.45	1.0-2.0	0.3-1.0	0.5-1-5
Temperature	°C	60-90	50-80	700-900	50-70
Pressure	bar	≤30	≤50	≤15	≤35
Footprint	m^{2} MW^{-1}	63	14.5	-	-
CAPEX	Euro MW^{-1}	800-1,500	1,400-2,100	≥2000	-
OPEX	%$_{\text{CAPEX}}$ a^{-1}	2-3	3-5	-	-

For more detailed information on the various electrolysis technologies, it is referred to the literature. Buttler and Spliethoff published a comprehensive overview of the technological fundamentals and KPIs of AEL, PEMEL, and SOEL [49]. A study by Smolinka et al. shows the state of the art of electrolysis technologies and prospective improvements based on direct communication with technology providers [52].

For further background and historical information, it is referred to the books of Schmidt, Kurzweil and Dietlmeier, and Smolinka and Garche [43,61,65].

2.2.2 Carbon Capture and Utilization

Carbon dioxide capture can be realized by a large variety of technological concepts and strongly differs with the applied source level, which is typically distinguished between ambient air and point sources with higher CO_2 concentrations, e.g. industrial flue gas streams. Furthermore, a differentiation between biogenic and fossil-based CO_2 sources is useful in the context of an environmental impact assessment of subsequent utilization processes [66]. Whereas utilizing biogenic or atmospheric CO_2 for synthetic fuel production creates a closed carbon loop, fossil-based CO_2 utilization merely represents a carbon recycling process with subsequent emissions from the fossil source once the synthetic fuel is combusted. However, even though ambient air provides a rather inexhaustible CO_2 source, separation is comparably energy-intensive due to the low CO_2 concentration of only 0.0407 vol.-% [19]. Point sources, on the other hand, provide CO_2 streams with high concentrations, dependent on the initial process characteristics, e.g. combustion of carbonaceous energy carriers for energy production or industrial processes such as steel making, steam methane reforming, and cement production [67].

CO_2 capture from point sources can be realized via three major processes, which are classified as pre- and post-combustion, as well as oxyfuel combustion [68]. At pre-combustion, gasification of fuels is applied to yield hydrogen for the combustion process and highly concentrated CO_2, which is usually captured via physical absorption or adsorption. At oxyfuel combustion, pure oxygen is applied for the combustion of carbonaceous fuels, leading to the exclusion of nitrogen and significantly lower flue gas volumes, which basically consist of CO_2 and H_2O. Thus, CO_2 can easily be separated via the condensation of water vapor [69]. At post-combustion processes, CO_2 is sequestered from flue gas streams. These consist of relatively low CO_2 concentrations due to the application of ambient air as the oxidant in the combustion process and thus high concentrations of nitrogen. However, as a significant advantage the post-combustion process can be retrofitted to existing plants, and large-scale applications were already realized. Generally, a large variety of technologies is applicable for post-combustion carbon capture, although chemical absorption is the most mature and widespread process [70]. Liquid sorbents are typically applied as washing agents to separate CO_2 from flue gas. Although a large variety of sorbents is available, monoethanolamine (MEA) is the solvent used most frequently in case studies that can be found in the literature [71].

Direct air capture (DAC) processes are mainly classified into high- and low-temperature technologies and have a comparatively young application history. Until 2019 15 DAC plants were in operation worldwide. The furthest developed technologies use either a liquid or solid solvent. Both approaches require thermal energy for the regeneration of the sorbent and for the release of the previously bound CO_2 compounds, as well as electrical energy, which is mainly required for the operation of fans [72,73].

In the liquid solvent-based high-temperature technology, gaseous CO_2 is absorbed by a strong alkaline hydroxide solution. An occurring anionic exchange leads to calcium carbonate precipitation. To recover the captured CO_2 from calcium carbonate high temperatures are required. A yield of one ton of CO_2 requires 1,420-2,250 kWh of thermal energy and 366-764 kWh in the form of electricity [19].

The most prominent technology provider is Carbon Engineering, which applies a potassium hydroxide-based approach coupled with a calcium caustic recovery loop. The company operates a pilot plant at its headquarter in British Columbia, Canada, and has a large-scale plant to capture 1 $Mt_{CO2}\ a^{-1}$ in the planning with a start of construction in 2022 [74].

In the solid sorbent low-temperature technology, porous cellulose-based and amine-supported materials are applied to capture CO_2 via weak intramolecular forces (physisorption) or strong covalent bonding (chemisorption). Fans push air through the contactor, leading to adsorption of CO_2 at ambient conditions. Once the sorbent is saturated, the process is switched from adsorption to a desorption mode, where residual air is evacuated via vacuum pumps. Furthermore, thermal energy at a temperature level of 100 °C is applied to release CO_2 and H_2O and regenerate the sorbent material [75]. Climeworks (Switzerland) and Global Thermostat (USA) are prominent technology providers and operate several demonstration plants. Maximum plant capacities currently operated by both companies are in the range of 4 $kt_{CO2}\ a^{-1}$ each. Moreover, Climeworks communicated the target of 225 Mt_{CO2} being removed from ambient air by 2025, leading to an overall energy consumption of approximately 297-518 TWh, according to the KPI data in Table 2.2 [72].

Table 2.2: Overview of key performance indicators of advanced carbon capture technologies. Data is based on [18,19,76–78].

Category	**Unit**	**DAC (low-temperature)**	**Post-combustion with MEA**
TRL	-	9	9
Technology provider examples	-	Climeworks, Global Thermostat	Shell, Mitsubishi Heavy Industries
Electricity demand	$kWh\ t_{CO2}^{-1}$	150-300	12
Heat demand	$kWh\ t_{CO2}^{-1}$	1,170-2,000	1011
Temperature	°C	≤100	≤140
Footprint	$m^2\ (t_{CO2}/a)^{-1}$	0.1	0.01
CAPEX	Euro $(t_{CO2}/a)^{-1}$	598	123

Details on DAC processes, specific technologies, and potentials are provided by Fasihi et al. and McQueen et al., while for further details on CO_2-capture from point sources it is referred to Fischedick et al. and Rubin et al. [19,71,79,80].

2.2.3 Hydrocarbon Synthesis

Hydrocarbon synthesis can be categorized into three subprocesses: (1) synthesis gas processing and conditioning, (2) conversion of synthesis gas into hydrocarbons, and (3) product upgrading [81]. This work considers hydrocarbon synthesis via chemical processes only.

Synthesis gas (syngas) technically describes a gaseous mixture consisting mainly of CO and H_2 beside low volumes of CO_2 and water vapor as well as potential detrimental trace element contaminations e.g. by nitrogen-, chlorine- and sulfur-compounds. At conventional synthesis gas production, e.g. based on coal, further purification is consequently required. Alternatively, CO_2-based syngas can be applied, consisting of CO_2 and hydrogen only [81].

For hydrocarbon production, synthesis gas is usually conditioned via reverse water-gas shift (RWGS) reaction to yield a specific H_2:CO ratio. This step is necessary for low-temperature Fischer-Tropsch (LTFT) synthesis, which lacks water-gas shift activity. High-temperature Fischer-Tropsch synthesis (HTFT) as well as methanol synthesis feature water-gas shift reactivity, enabling direct hydration of CO_2 without further conditioning. The Sabatier process for methane production features both, fuel synthesis via CO_2 as well as via CO [82][21].

Within LTFT synthesis, mainly linear chained hydrocarbons (simplified representation as -CH_2- in Equation 1 and Equation 2) in the range from methane to long-chained hard waxes are converted via exothermic reactions:

$$CO + 2H_2 \rightleftharpoons (CH_2) + H_2O \quad \Delta H_R = -154 kJ/mol \tag{1}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \; \Delta H_R = \; -41 kJ/mol \tag{2}$$

In accord with high activity, stability, and selectivity, catalysts for industrial applications are usually iron- and cobalt-based, whereas noble metals such as ruthenium are typically avoided due to significantly higher costs [62]. The temperature range for the synthesis process is between 180-270 °C and influences the product spectrum. Higher temperatures lead to higher reaction rates and thus to a higher yield of hydrocarbons. In contrast, average chain lengths decrease with higher temperatures, leading to a shift in the product composition. Further process parameters influencing the product composition are the synthesis gas ratio, space velocity, and pressure level. Typical reactor types for industrial-scale applications are tube bundle reactors beside bubble column reactors. R&D focuses on new catalysts and enhanced reactor types such as micro- and nano-structured fixed-bed reactors [72].

HTFT is conventionally carried out in fluidized-bed reactors and based on iron catalysts. Process temperatures are typically in the range of 300-350 °C and synthesized hydrocarbons are rich in gasoline and olefins. Further R&D focuses on an improved water-gas shift activity besides a better CO_2 conversion [83,84].

Methanol synthesis is a mature technology, with methanol being an important platform chemical for various industrial applications. Global demand vastly increased over the last decade and is expected to reach up to 500 Mt a^{-1} by 2050 compared to 107 Mt a^{-1} in 2021 [85,86].

Methanol can be synthesized either via conventional synthesis gas or directly via CO_2 hydrogenation:

$$CO + 2H_2 \rightleftharpoons CH_3OH \;\; \triangle H_R = -91 kJ/mol \tag{3}$$

$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \; \triangle H_R = -49 kJ/mol \tag{4}$$

Due to the exothermic reactions, low process temperatures are thermodynamically beneficial. Comparatively high pressures in the range of 50-125 bar are applied to achieve maximized product yields. Metal-oxides based on Cu and Zn are commercially utilized catalysts [72]. The process based on synthesis gas achieves a higher conversion of 50-80 % per pass compared to approximately 35 % for direct CO_2 utilization. However, recycling streams can be easily applied. The synthesis of CO_2-based feeds was demonstrated in several projects with the George Olah plant in Svartsengli, Iceland, being the first commercial plant commissioned in 2012. The methanol selectivity is higher for the CO_2-based process with a very low content of by-products beside water [16,87].

Methanation is a special case of the Fischer-Tropsch reaction with a low chain propagation probability. The exothermic chemical reaction takes place at 250-475 °C:

$$4H_2 + CO_2 \rightleftharpoons CH_4 + 2H_2O \; \triangle H_R = -165 kJ/mol \tag{5}$$

Ni catalysts are typically applied beside other configurations based on Ru, Fe, Co, and Pt. A challenge for all reactor types is adequate heat dissipation to reach a high product yield and avoid catalyst damage. Methanation plant scaling is rather flexible and dynamic operation is possible with a lower part load limit of 50 % [88–90].

For detailed insights into the different paths and concepts of hydrocarbon synthesis, it is referred to Maitlis and de Klerk regarding Fischer-Tropsch synthesis. In the comprehensive book of Behr et al., detailed information on methanol synthesis is provided, while the technical concept of methanation is described by Ghaib [21,85,91].

2.2.4 Upgrading

The process chain of PtF concepts is usually portrayed with a focus on electrolysis, carbon capture, and hydrocarbon synthesis. However, depending on the process route, further product upgrading may be required. This applies especially to the Fischer-Tropsch synthesis route. Hydrogen and methane usually require gas drying and conditioning for further application [49,92]. Methanol requires separation and purification prior to a utilization as platform chemical or as feed for the production of fuels. Hydrocarbons produced via Fischer-Tropsch synthesis instead rather contain a broad product mix with different chain lengths and are often referred to as *syncrude*, analogous to crude oil. They cannot be directly applied as drop-in fuels and require further upgrading [20]. To achieve fuels that meet specifications and chemicals, a fractionation into corresponding boiling ranges and chain lengths has to be applied via distillation, among other processes [21]. Light fuel gases (C_5/C_6), naphtha ($C_{7\text{-}10}$), middle distillates ($C_{11\text{-}19}$), and waxes (C_{20+}) are considered relevant fractions in the context of fuel upgrading. For naphtha and middle distillates, olefins are hydrated to paraffines via hydrotreating to achieve heating value and octane number enhancements. Within hydrocracking, the wax fraction is converted to naphtha and middle distillates. The octane number of light fuel gases, which also evolved from the hydrocracking process, is increased via catalytic isomerization. A catalytic reformer is applied to increase the octane number of naphtha and for the production of aromatic hydrocarbons [93].

By this means, for PtF plants with Fischer-Tropsch synthesis, a strategy for *syncrude* treatment is required. This can be realized via *syncrude* transport to conventional refineries for subsequent upgrading via co-processing. However, a blend of *syncrude* to conventional crude oil refining is limited according to deviant product specifications. Hence, co-processing should apply as an intermediate process towards a sustainability-orientated transformation of refineries on the one hand (cf. Appendix B). On the other hand, for rather decentralized PtF concepts, (partial) refining including at least distillation and hydrocracking should be considered as part of the PtF plant. For fully decentralized approaches, all of the above-mentioned processes should be applied. In the short term, this could be realized via modular container-based solutions as already demonstrated in small-scale.

Detailed information on *syncrude* upgrading processes is available in the textbook of Maitlis and de Klerk, while the work of König et al. and Becker et al. provide techno-economic parameters of the respective upgrading technologies [20,21,93]. A further discussion of viable *syncrude* upgrading process routes is carried out in Schnuelle et al. in Appendix B.

Chapter III

3. Methodological Approach and Data Acquisition

With the three central research questions and the initial hypothesis in mind, this dissertation addresses a variety of scientific disciplines. While the major research focus evolves from the field of engineering sciences, strong linkages to economics, social sciences, and politics need to be taken into account as well. The approach of combined socio-techno-economic analyses allows covering the relevant interdisciplinary aspects of both, energy system transitions as well as the study of *system innovations* such as PtF. According to Fischedick et al., *system innovations* can only sustainably contribute to a successful energy system transition, if non-technical but rather societal and infrastructural requirements are fulfilled besides the presumed provision of technical system services [11]. Consequently, the common energy system-related approach of techno-economic analyses is complemented by socio-technical and socio-economic perspectives and merged into an integrated analysis of implementation strategies for PtF concepts in Germany.

Within each publication in Chapter VI-Chapter IX, the individually applied methodologies are described in detail. The following subchapter provides a holistic overview of the strategic background of the chosen methodological approaches. Furthermore, a brief overview of supplementary methodologies, which are applied in the accompanying publications of Appendix A and Appendix B, is provided. In addition, a reflection of the applied procedures for data acquisition is addressed in Subchapter 3.2.

1.3 On the Necessity of an Interdisciplinary Investigation Approach

From a technical perspective, energy technologies provide harmonized services to ensure a constant energy supply. A further overlapping dynamic, however, occurs on a societal level through markets, political decision making, and central stakeholders from commerce, industry, civil society, and science [94]. Research on energy systems should take this into account and thus follow multi- and interdisciplinary investigation approaches. According to Cherp et al., several kinds of changes apply to energy system transitions. First of all, a shift in energy production and consumption occurs. Secondly, technologies for the extraction, transformation, and utilization of energy change. The third change is related to policies regulating the energy system, e.g. to achieve modernization, increase national independence, or mitigate environmental damages and climate change. Cherp et al. classify the three types of changes as techno-economic systems, socio-technical systems, and systems of political actions, co-evolving with one another. Although these systems consist of individual boundaries, elements, and connections, they can hardly be analyzed apart from each other in the context of energy system transition research [95].

Within the techno-economic perspective, a technical assessment of technologies, processes, and innovations is carried out with an integrated economic investigation to determine functionality, advantages, and disadvantages besides economic competitiveness in energy markets. However, questions concerning the emergence and diffusion of technologies are out of scope. The socio-technical perspective has a more complex view on technologies and innovations. It rather reflects them as a social phenomenon that interacts with stakeholders and within social networks – thus in socio-technical (energy) systems. In line with this approach is the popular socio-technical transition analysis model called ‘Multi-Level-Perspective’ (MLP), developed and enhanced by Geels et al. [96–98]. The MLP focuses on innovations that occur outside dominant regimes and evolve in small niches until they might become mature and competitive enough to enter the markets and established regimes. The latter need external destabilizing impacts to overcome the established internal regime resilience, e.g. political regulations to enforce structural changes (cf. Section 3.1.2 and Chapter VIII). Within the political perspective, national governments, i.e. the ‘state’, play a central role in analyses and are not just interpreted as ordinary (economic) actors or external ‘landscape’ factors. They can pursue national interests, e.g. economic growth and increasing employment, but also special interests such as the transition towards renewable energies [95].

Based on this information, it can be derived that a plurality of methodologies from different disciplines is required instead of one single approach to sufficiently address the three central research questions. The individual methodological approaches carried out in this work are briefly discussed in Section 3.1.1, Section 3.1.2, and Subchapter 3.2. Nevertheless, in contrast to the above-described classification into techno-economic, socio-technical and political perspectives, the approach is merged into a socio-technical and a socio-economic perspective. This accounts for the underlying understanding that the analysis of technical functionality and economic competitiveness needs to be considered in relation to the provision of specific system services for the socio-technical energy system on the one hand. Furthermore, the techno-economic potential is strongly dependent on the progress of the overall transition progress of the socio-technical energy system, since PtF concepts are only useful at high RE shares. On the other hand, the integration potential into the socio-technical energy system is dependent on socio-economic relations with clearly defined stakeholders representing various fields of society. In addition, a successful large-scale PtF integration will cause economic short-, medium- and long-term impacts for both, individual customers as well as for the national economy and is thus further justifying a socio-economic classification.

3.1.1 Investigations from a Socio-Technical Perspective

In a first published paper, an overview of basic characteristics in the fields of technical fundamentals and specifications is provided. It is accompanied by a review on societal acceptance of PtF concepts (cf. Chapter VI). The work is based on an extensive literature review and is crucial to achieving a comprehensive understanding of the state of the art of individual technologies and specific PtF configurations. For all further investigations, an initial distinction is made between centralized and decentralized PtF concepts with their specific related system services. Accordingly, the general technical qualification of water electrolysis and hydrocarbon fuel synthesis for dynamic operation modes as well as limitations of plant capacity up- and down-scaling are discussed. In addition, implications of the availability of scarce catalyst materials are investigated concerning expected global demand and resources, respectively. Furthermore, implications on water, $CO_{2,}$ and renewable energy availability are investigated in the context of scenario-based future PtF capacity expansions. A first link to the topic of socio-economic aspects is carried out by a brief investigation of economic correlations to fossil fuel markets. Based on the work published in Chapter VIII, production costs of synthetic fuels are calculated according to specific techno-economic assumptions and energy market regulations. Based on these findings, the impacts of a broad PtF integration in Germany are discussed with respect to the national economy. Here, a semi-quantitative approach is carried out to determine the resulting environmental impact costs of an ongoing fossil fuel supply compared to the substitution costs of natural gas and crude oil-based products by electrolytic hydrogen or synthetic fuels. The gained knowledge is furthermore applied to a discussion regarding the contributions of PtF concepts to a more resilient energy supply.

A follow-up publication focuses on the question of technical limitations regarding dynamic operation modes in detail. To date, there is no long-term experience for such operating concepts, and techno-economic assessment studies are rather generalized without considering the technical limitations of electrolyzers in dynamic operation in detail. For an improved understanding, an electrolysis model was developed to enable a profound assessment of hydrogen production with fluctuating electricity feed-in. It allows a consideration of ramp speed limitations and specific plant characteristics at partial load operation of both commercial LT electrolysis technologies, AEL and PEMEL. Electrochemical fundamentals of AEL and PEMEL electrolysis stacks, as well as relevant plant periphery, i.e. power electronics, pumps, and gas dryer, are implemented into a newly compiled simulation tool based on recent literature (Figure 3.1). Simulations are carried out for onshore and offshore wind farms and a west-east orientated PV plant, all located in northwest Germany. The techno-economic assessment covers considerations of specific electricity procurement costs for the individual power sources besides maintenance costs according to the modeled operating patterns.

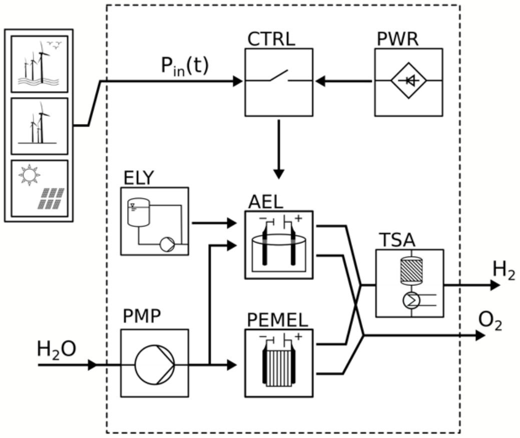

Figure 3.1: Schematic model structure representing the major components of electricity and water feed-in management and the AEL and PEMEL stacks with respective electrolyte pumping and gas drying (cf. Chapter VII). CTRL – control, PWR – power, ELY – electrolyte pumping, PMP – pump, TSA – temperature swing adsorption.

Mathematical equations in terms of the actual electrochemical relations are applied for quasi-dynamic modeling of the electrolyzers' operating behavior. In this context, the term "quasi-dynamic" describes an approximation of the dynamic behavior through a static calculation of small time increments and dynamic temperature relations, while applying fluctuating electricity feed-in signals. The model components are implemented in python 3.7. The approach enables the utilization of different electricity feed-in time-series sets with a simulation period of one year. Besides this long simulation period, the innovation of this approach lies in the merging of electrochemical relations for a representation of the cell performance with a previously published temperature model and a concurrent consideration of the plant periphery. Modeling of the underlying electrochemical fundamentals is based on published models in the literature. All details on the model setup and specific electrochemical background information are provided in full length within Chapter VII.

3.1.2 Investigation from a Socio-Economic Perspective

Investigations regarding integration pathways of PtF into the German energy system are carried out based on the utilization of two models emerging from innovation theory. One is the above-mentioned MLP from Geels et al. According to the MLP, system innovations like PtF can destabilize existing regimes (e.g. the energy system as a whole or specific parts of it) and evolve a systematic and guided change of mature structures. At current state, PtF may still be interpreted as niche innovation, which can emerge from the niche into the mainstream markets – or fail. Several so-called *impact factors* influence the direction of innovation processes towards success or failure. They derive from a complex overlapping dynamic between markets, political decision-making, central stakeholders from commerce, industry, civil society, science, and technological change, as well as unforeseeable incidents [99–102]. These MLP-related impact factors are specified with the "turtle model of guiding impact factors" (turtle model). It allows for a qualitative discussion and visualization of the drivers influencing innovation direction and the specific role of these different impact factors (cf. Figure 3.2) [101,103–108]. The core of the model displays a network of participants in the innovation process. Yet, primarily entrepreneurs and progressive companies are the major actors in this young environment. They built and operated the first pilot plants, assisted by research institutes and governmental funds. Furthermore, participating actors formed strategic networks to push the development forward and support the introduction of desirable legislation. The six impact factors can be distinguished into *push* and *pull* factors. While *push* factors have the ability to destabilize existing regimes and create new space for innovations, *pull* factors unfold selective effects and promote the innovation process. All details on the turtle model are provided within Chapter VIII.

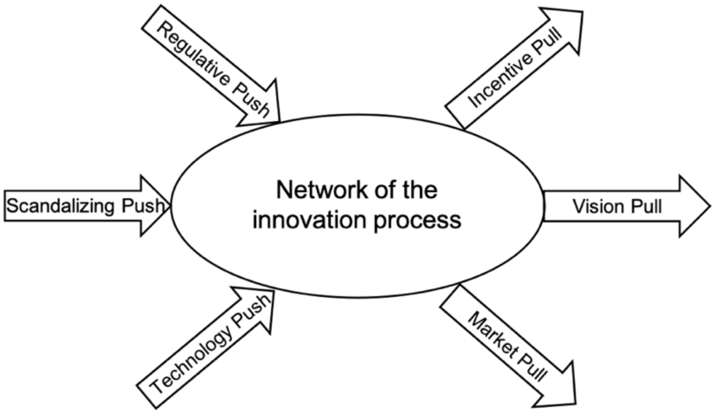

Figure 3.2: Turtle model's basic setup – an internal network of stakeholders is influenced by several *push* and *pull* factors (cf. Chapter VIII).

The application of these models requires both, accumulated knowledge about technical characteristics and information on the innovation system of PtF technologies (cf. [108,109]). Information and data are obtained from literature, but also from stakeholder dialogues to achieve an in-depth understanding of specific interest groups (cf. Subchapter 3.2). The gained knowledge is related to the turtle model and structured accordingly. However, more complex interrelations between actors and their environment are not included, and a dynamic investigation of the innovation system's development over time is impossible with this approach. A significant methodological improvement carried out within this dissertation is thus a translation of the turtle model into a simulation tool. For this purpose, a deterministic agent-based model was developed. The concept of agent-based modeling (ABM) allows for an intuitive implementation of important stakeholder characteristics in conjunction with dynamic framing conditions [110]. As it was found in a collaborative study with Holtz et al., ABM can be very supportive for generating transformation knowledge in the context of energy system transitions [111]. The newly developed model simulates the situation depicted in Figure 3.3 and allows for a quantitative analysis of both, representative stakeholders with their specific interests as decision-making agents as well as a defined environment, i.e. the German energy markets with all relevant characteristics concerning participants, prices and sales volumes. This way, the model enables to investigate the uptake *from niche to market* of PtF concepts, given the various actors and *push* and *pull* factors from the turtle model. It revolves around investment decisions made by PtF plant operators and purchasing decisions made by customers, all within a dynamic context of evolving regulation and technological progress.

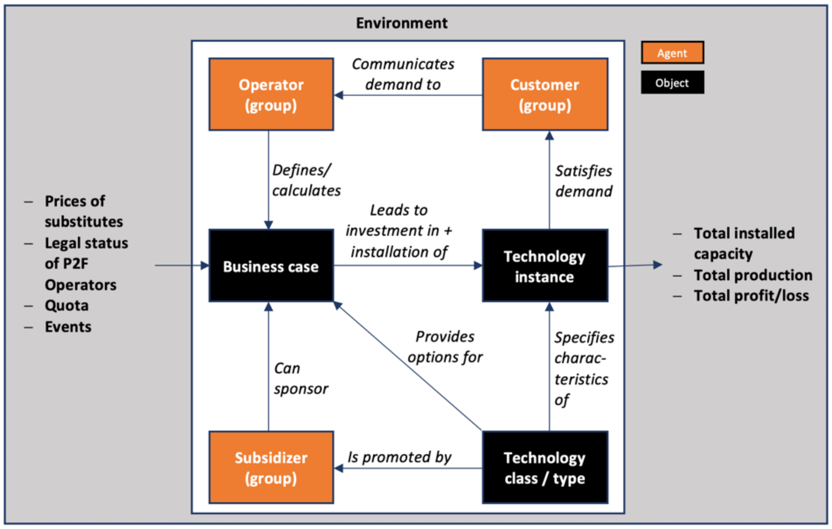

Figure 3.3: Schematic model setup – Active agents (orange) are separated into operators, customers, and subsidizers, while different technologies and related business models are central objects that interact with the agents.

Active agent types are operators, customers, and subsidizers, representing a whole group of agents who together are considered as individuals. In addition, the model includes technology classes, (installed) technology instances, and individual business cases as passive object types. The model environment provides the regulatory and economic context for the interaction of agents and objects. For validation purposes, the underlying model setup was discussed with stakeholders from the field (cf. Subchapter 3.2). A detailed description of the model's functionality and characterization is provided within Chapter VIII.

Within a follow-up publication, another socio-economic focus is put on the economic consequences of a broad PtF diffusion for German customers and the economy. In a nutshell, price developments of conventional fuels and their renewable substitutes are observed until 2050. They are discussed in comparison to historical price dynamics and under consideration of actual societal energy expenses, including environmental impact costs of specific energy carriers. While a development or enhancement of methodological approaches was out of scope in this study, it instead stresses the divergence between widespread public perception and statistical data. The goal of this research is to sensitize critics of the energy system transition and disclose the frequently misleading price debates in several media formats. Applied methodological tools involve reviewing literature and statistics, statistical data processing and migration into own databases, and calculation of real prices based on standard procedures.

3.2 Accompanying Application of Further Methodologies and Data Acquisition Approaches

Techno-economic analyses (TEA) were carried out for both, single technologies as well as whole process chains of PtF concepts. The methodological approach is continuously based on the standards published by Peters et al. and with adaptations according to Koenig et al. and partly own modifications [20,112]. All costs are classified either as capital expenditures (CAPEX) or operational expenditures (OPEX) throughout the four publications of Chapter VI-Chapter IX. For all technologies, capital-related costs are calculated according to published reference costs for a reference plant capacity via an applied scaling factor. Based on this so-called purchased cost of equipment (PC), the fixed capital investment (FCI) is calculated by multiplying the PC with a ratio factor (RF). The FCI represents the sum of direct and indirect capital investment costs. The applied RF includes costs for installation, instrumentation, piping, electrical systems, buildings, yard improvements and service facilities, engineering, construction, legal expenses, and contractor fees. Especially in the case of electrolyzers, which are usually supplied as skid-mounted units, several of these costs do not apply and RF is reduced accordingly. Annualized CAPEX (ACAPEX) are based on the FCI under consideration of a specific plant lifetime and an assumed interest rate. The OPEX consider service and maintenance, insurances, taxes, materials, utilities, and in the case of electrolysis stack replacements, electricity supply and supply with deionized water. The total number of stack replacements required per system lifetime depends on the annual operating hours. A novel approach carried out in Chapter VII is the calculation of stack replacement costs according to the specific operation mode. This procedure is based on the simulated operating patterns of LT electrolyzers with direct RE supply and ensures that dynamic operation is also considered in the TEA. The net production costs (NPC) are calculated based on the product of ACAPEX and OPEX divided by the annual product output.

Another methodological approach for comparing different technology options is the multi-criteria decision analysis (MCDA). Within an accompanying publication of this dissertation, an MCDA for LT electrolysis and CO_2-capture technologies was carried out to identify the best technology options for a specific case study (cf. Appendix A). The approach allowed for a detailed comparison under consideration of ecological aspects besides techno-economic parameters. This can be considered crucial in the light of the general motivation for PtX plants: a contribution to low GHG emissions and environmental impacts. While there is not the one and only methodological procedure for MCDA but rather a large variety of different approaches, the well-established methods of the Analytical Hierarchy Process (AHP) and the Weighted Sum Model (WSM) are applied. The carried out procedure is described in detail within the respective publication in Appendix A.

A central task within the dissertation project was the acquisition of appropriate data. Especially in the context of the agent-based model development, comprehensive information and data input from stakeholders were required to better understand and calibrate the individual agents adequately within the model. To do justice to this, a stakeholder workshop with representatives from the PtF network was organized. Besides the presence of plant developers and operators, also enterprises representing potential customers of PtF products participated. In addition, an interdisciplinary delegation of researchers took part as well. The following companies and institutions were present:

- Audi AG
- Bertrand AG
- dena GmbH
- Entwicklungsagentur Region Heide AöR
- EnviTec Biogas AG
- Fraunhofer IFAM
- Fraunhofer IWES
- IKEM – Institut für Klimaschutz, Energie und Mobilität – Recht, Ökonomie und Politik e.V.
- IÖW – Institut für ökologische Wirtschaftsforschung GmbH
- MicrobEnergy GmbH/ Viessmann Group
- Projektträger DLR
- Projektträger Jülich
- Reederei AG EMS
- RWTH Aachen
- SGS Germany GmbH
- Sparkasse Bremen AG
- Sunfire GmbH
- Delft University of Technology
- Eindhoven University of Technology
- Universität Bremen
- Rijksuniversiteit Groningen
- Wpd Onshore GmbH & Co. KG
- Wuppertal Institut GmbH

The presentations and discussions from the participants were essential for the model-building process. Especially insights on the strategic investment decisions enabled a differentiated implementation of the respective PtF operator agents. The same applies to the implementation of specified customer groups. A collective statement of the group was that funding plays a significant role and is awaited to be of the highest importance in the short- and medium-term for PtF integration. Accordingly, a heightened effort to adequately implement specified funding mechanisms into the model was applied.

In addition, the list of relevant parameters for all calculations is long and literature values often strongly deviate, especially technology KPIs. Besides individual approaches of sensitivity analyses, the applied data was partly orientated to the work of the data harmonizing project “BEniVer” within the funding line “Energiewende im Verkehr” of the Federal Ministry of Economics and Climate Affairs [113]. This procedure enabled two benefits. On the one hand, chosen parameters in this work can be considered reasonable, since they are double-checked by another institution. On the other hand, a better consistency with work from other researchers in the field is accomplished.

Chapter IV

4. Major Results

This chapter provides an overview of the essential results of the dissertation project. In the first instance, the key findings of each paper are presented and merged in the context of the socio-technical and socio-economic perspectives. This includes both, the publications of Chapter VI-Chapter IX as well as the two accompanying papers provided in the Appendix. The central results of each work are summarized and restructured within Subchapter 4.1 and Subchapter 4.2. For further details and a more differentiated view, it is referred to the corresponding Sections within the underlying papers. An in-depth discussion of the compiled results in a broader scientific context follows within the Conclusion in Chapter V.

4.1 Outcomes from Socio-Technical Analyses

The material and energy flow analyses of Chapter VI showed that water demand for electrolysis can be considered rather uncritical, at least in Germany by now. It was revealed that 450 million liters or 450,000 m^3 of water are required per TWh of produced hydrogen. Annual total water demand in Germany is valued at 25.1 billion m^3 in contrast, whereas the potential water supply is stated as high as 188 billion m^3. However, despite these vast water sources, increasing water loss is an upcoming issue in Germany, resulting in temporal water scarcity in several regions. By this means, a drastic annual loss of approx. 2.5 billion m^3 was registered for recent years, which is among the highest values worldwide [114]. These findings emphasize the requirement of appropriate recycling streams of wastewater. Along PtF process chains, this applies especially for CO_2-capture and hydrocarbon synthesis. But also within the utilization of hydrogen for other processes, e.g. steel production via the low carbon process route of direct reduced iron (DRI-route), vast amounts of water are generated as a side product.

CO_2 is required as educt for the production of hydrocarbon-based fuels. Whereas different carbon sources are discussed in Chapter II, the actual demand for PtF depends on the chosen scenario. Based on the molecular weights of CO_2 and methane and related to the energy content of methane, 0.2 t_{CO2} are required to produce 1 MWh_{CH4}. For a discussed scenario in Chapter VI, a methane demand of 55 TWh equals a requirement of 11 Mt_{CO2}. For the production of synthetic liquid fuels, the actual CO_2 demand is dependent on the hydrocarbon chain lengths. Recent studies suggest 0.27-0.34 t_{CO2} for 1 MWh of *syncrude*. In an extreme case scenario for a greenhouse gas neutral energy supply in Germany, 552 TWh of synthetic fuels are projected for 2050, involving a corresponding CO_2 demand of 149-187.7 t. The latter is far beyond national biogenic CO_2 sources.

Availability of scarce materials is found to be critical for PEMEL, which requires platinum group metals, e.g. platinum, ruthenium, and iridium, on both electrode sides. R&D on PEMEL focuses on alternative catalyst materials and lower cell area-specific demand. Nevertheless, the calculations carried out in Chapter VI revealed a platinum demand of 10 t for PEMEL cathodes at an installed capacity of 100 GW_{el}, equaling 4.6 % of global platinum demand in 2015. In contrast, AEL technology is not facing any potential material supply bottlenecks with nickel as the standard catalyst material. For methanation, nickel is the common catalyst of choice either. Expected demand for both, AEL as well as methanation can be considered uncritical even at large global capacities. In contrast, ruthenium provides a better activity. It is regarded as an alternative catalyst for the Sabatier reaction as it can enable both, a more dynamic operation of the methanation process as well as higher conversion yields. The latter allow for shorter reactor lengths, reducing the steel demand and thus capital expenditures. For Fischer-Tropsch reactors most relevant catalyst elements are iron, cobalt, and ruthenium. In Chapter VI, it is stated that a Fischer-Tropsch reactor equal to a 5 GW plant capacity requires 200 t of active catalyst material, which is negligible for iron and cobalt with regard to global reserves. However, cobalt prices increased drastically in the recent past, as global demand also grew significantly, e.g. for battery applications. Ruthenium is considered too expensive as the main material and can be considered critical even as a minor catalyst component of about 1 wt.-%. For the exemplary calculation, a resulting ruthenium demand of 2 t is significant related to global consumption of 34.2 t in 2016.

Both considered synthesis processes, methanation and Fischer-Tropsch synthesis, feature a limited dynamic operation capability. The actual flexibility potential is mainly correlated to the activity of catalyst materials. Whereas the commonly utilized elements provide relatively low activity, noble metals can be considered critical in price and availability. A further challenge by this means is an appropriate heat management of the strongly exothermal reactions and product quality. Whereas the *syncrude* composition from Fischer-Tropsch synthesis may change at dynamic operation modes and cause higher efforts for subsequent upgrading, the conversion yield at methanation might deteriorate and induce higher methane purification efforts.

Concerning electrolysis, literature often stresses a comparatively poor performance of AEL in dynamic operation compared to PEMEL. However, AEL achieved considerable progress in recent years (cf. Chapter II). In Chapter VI, it is stated that further research is required in the field of investigating dynamic electrolysis operation capability.

Hence, the follow-up publication of Chapter VII features a comparison of AEL and PEMEL regarding dynamic operation modes according to RE production patterns. The functionality of the AEL and PEMEL models could be approved, as stack temperature and cooling-water flow follow an expected trend according to the underlying power input. In addition, product gas balances show a molar hydrogen/oxygen ratio of 2:1 with a proportional trend to the current density and power input at the stack level. A case study considering a direct PV power supply shows the much better capability of PEMEL regarding electricity utilization. At the considered plant setup, PEMEL utilizes 97.3 % of the supplied electricity from the PV farm and accumulates 3,111 operating hours per year, whereas AEL achieves an utilization rate of 84.7 % with only 1,868 operating hours. Nevertheless, corresponding full load hours (FLH) and hydrogen yield show only a small gap with 4.39 t_{H2} a^{-1} (1,148 FLH) for PEMEL compared to 4.02 t_{H2} a^{-1} (1,004 FLH) for AEL. These results reflect the higher ramping speed and lower part-load operation capability of PEMEL. In contrast, in terms of economics it is revealed that the higher utilization rates of PEMEL can be even unfavorable. This applies for example for the case study considering electricity feed-in from a “modern” onshore wind farm. Thanks to the dynamic TEA as portrayed in Chapter III, stack overhaul costs related to actual operating hours could be investigated. Due to the shorter stack overhaul period for PEMEL and the higher operating hours, two major stack overhauls are required over the electrolysis system lifetime compared to only one for AEL. A corresponding cost breakdown for AEL and PEMEL hydrogen net production costs is displayed in Figure 4.1.

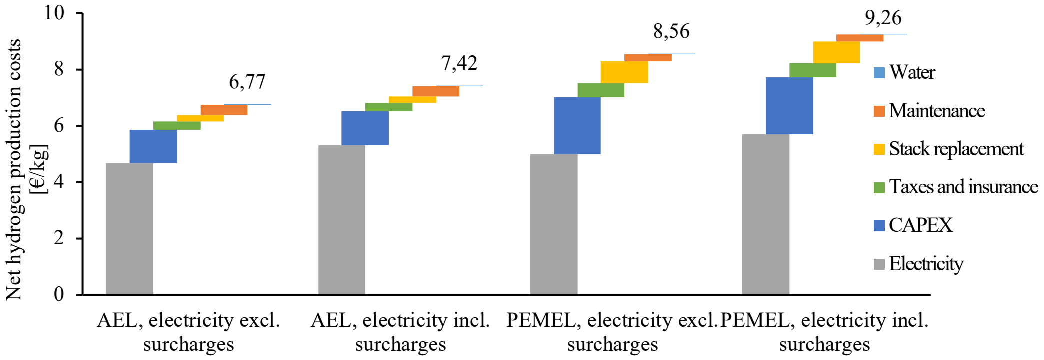

Figure 4.1: Net hydrogen production costs breakdown with electricity feed-in of a “modern” onshore wind farm.

Although electricity procurement costs with or without additional surcharges have the highest impact on NPC, stack overhaul costs also correspond for 3.2 % in the case of AEL and 9.1 % in the case of PEMEL, respectively (3.0 % and 8.4 % including electricity surcharges).

Figure 4.2 shows the simulated utilization rates and average efficiencies for both electrolysis types at varying plant scaling configurations for all considered RE power feed-in signals. Two major implications can be derived from this depiction.

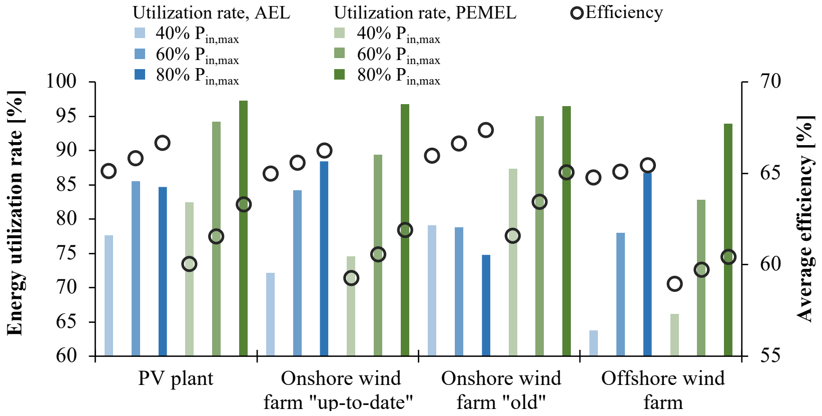

Figure 4.2: Comparison of simulated utilization rates of the various electricity feed-in signals at different electrolyzer scaling. Simulated average system efficiencies of AEL and PEMEL show an increasing trend with higher electrolyzer scaling.

On the one hand, efficiencies clearly improve with increasing plant scale, which is mainly correlated to more operating hours at lower part-load levels. In addition, the relative energy demand for plant periphery decreases. On the other hand, an increased electrolyzer scaling does not generally imply better utilization rates, as can be observed in the case of AEL in combination with the PV and “old” wind farm electricity feed-in.

Although the investigation was based on low-pressure electrolysis technologies, there is a controversial debate on pros and cons of high- (HP) versus low-pressure (LP) systems in the field of electrolysis R&D.

Whereas HP models do not require additional compressors for hydrogen storage or pipeline feed-in, the technology suffers from lower current efficiencies and stack lifetime and potential safety hazards due to a higher risk for product gas mixing among other drawbacks. On the contrary, LP systems operating at ambient conditions require further plant periphery in the form of compression stages, leading to additional investment costs, further energy losses, and increased complexity of the overall electrolysis system. In the MCDA carried out within the accompanying publication in Appendix A, HP and LP systems of AEL and PEMEL technology were analyzed. The investigation showed that for both, AEL and PEMEL, the LP configuration with subsequent compression could outperform the HP alternative due to better system efficiencies as well as lower maintenance and capital costs, among other factors.

A frequently discussed PtF use case is the application of surplus energy from wind and PV power, which is unavailable for the electricity sector due to grid congestions. At first glance, this operation concept is especially interesting from a socio-technical perspective, as a curtailment of RE and excessive electricity grid extensions could be avoided. Besides the unfortunate “loss” of energy, both issues raise acceptance problems of the energy system transition. However, even if the accumulated feed-in management exceeded 5.52 TWh in 2017 throughout Germany, local emergence of surplus energy appears very infrequently. The discussion in Chapter VI shows that PtF operation concepts focusing on surplus energy utilization can hardly be realized due to the very low operating hours of electrolyzers.

The investigation in Chapter VI also shows that social acceptance for PtF concepts is rather high until today. Stakeholders from pilot plants reported that they were not confronted with acceptance issues. Instead, the opposite has partly occurred as a fraction of private customers showed a higher willingness-to-pay for electrolytic hydrogen. This phenomenon is taken into account in more detail in the following Subchapter 5.2. However, acceptance problems could come up with a more extensive PtF diffusion in the context of the limited process efficiencies and significantly higher product prices compared to former conventional energy prices. Calculations showed that annual national expenses for liquid fuels and gas could treble if the conventional energy carriers are replaced by PtF products. Nevertheless, in the recent months, energy prices drastically exceeded any former price dynamics and caused significant disruptions for whole economies and global trade. Surprisingly, renewable energies suddenly achieve an increasing perception to be of central importance for stable energy prices besides supply security (cf. Chapter IX).

4.2 Outcomes from Socio-Economic Analyses

A central result of Chapter VIII is the transformation of the utilized turtle model with structured information on the internal PtF innovation system and on all external impact factors into the newly developed agent-based model (see Figure 4.3). Based on the gained understanding of basic market mechanisms and stakeholder motivations, all relevant information and interrelated contents could be successfully implemented into the model.

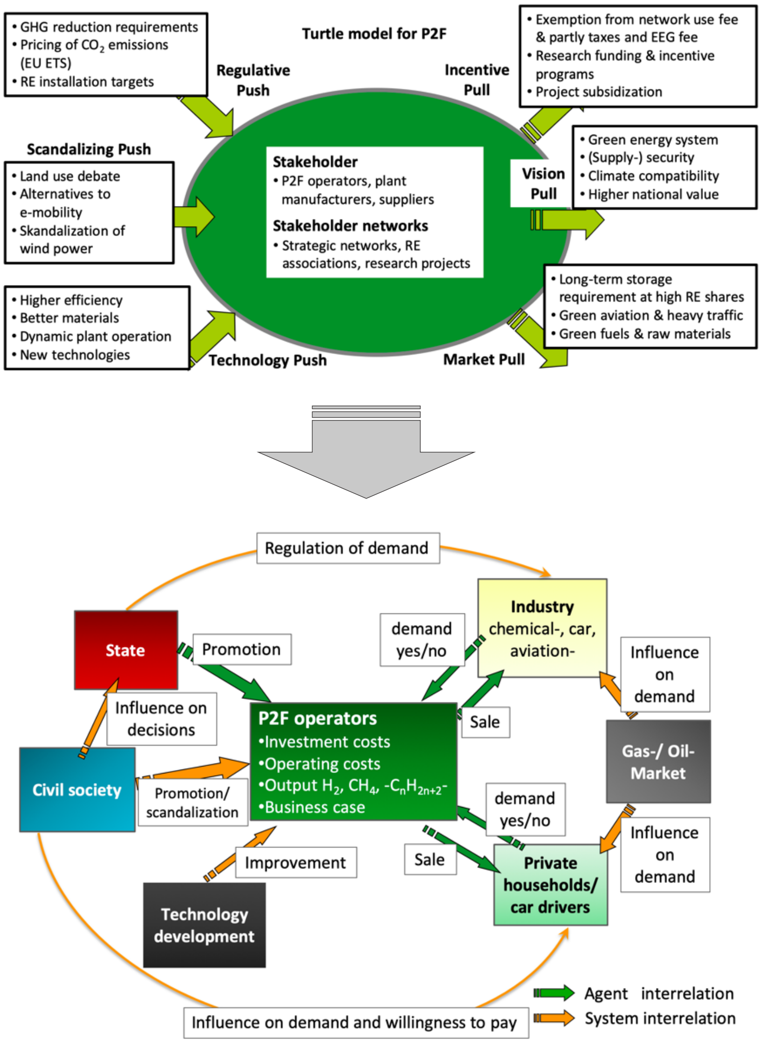

Figure 4.3: Transformation of the turtle model into the agent-based model. Relevant insights on the PtF innovation system collected within the turtle model is assigned to specific agents and objects, enabling a prospective investigation for ways out of the niche into the German energy markets (cf. Chapter VIII).

A simulation for calibration reasons showed valid results compared to actual developments in the respective time frame (2011-2016). This applies to accumulated installed capacities, the number of plants, and the share of private investments and public funding. Further proof concerning model validity can be derived from the time horizon between 2016-2020. While the calculated capacity for 2016 matched the actual installed capacity very precisely, the simulation also reflects the slow increase until 2020 with a result of 27 MW_{el} (compared to 25 MW_{el} in reality). Within a base scenario at constant framing conditions, the simulation shows a maximum installed capacity of 42 MW_{el} in 2029. The ratio of private investments and public funding to realize these PtF plants is nearly 1:1 and thus indicates the unfavorable economic conditions.

Further simulations showed that single adjustments to framing conditions hardly increase the economic viability of PtF concepts. Several modifications were introduced step by step for an investigation over the time horizon between 2016-2035. Linearly implemented price increments of 2 % a^{-1} and 4 % a^{-1} for conventional energy carriers do not show considerable effects. Even though an installed capacity of nearly 90 MW_{el} is achieved by 2035, the realized plants are strongly dependent on subsidization and generate structural financial losses during operation.

An exemption from the EEG (Erneuerbare-Energien-Gesetz, Renewable Energy Act) fee for electricity feed-in is doubtless beneficial in terms of PtF business case creation. It is the main component of electricity surcharges and was of central importance in debates between stakeholders and policy for years. Nevertheless, an exemption of PtF concepts from the EEG fee, as recently legally confirmed, will not be sufficient to embrace a rapid PtF rollout. However, a tipping point regarding the ratio of private investments and public funding is reached with a value of nearly 3:1 by 2035. The higher investments lead to an accumulated PtF capacity of 321 MW in 2035. The better but still low growth rate originates from a significant price gap between conventional fuels and the renewable substitutes.

Hence, in a more progressive scenario, additional energy policy adjustments are implemented. These include a high EU ETS (Emissions Trading System) certificate price of 100 € t_{CO2}^{-1}, strict GHG reduction quotas for industrial companies beside an intensified start-up subsidization of 60 M€ a^{-1} until 2025 for PtF projects. The results in Figure 4.4 show at first sight that a combination of multiple policy adjustments yields a significantly improved PtF rollout with an accumulated capacity of up to 4.4 GW_{el} in 2035.

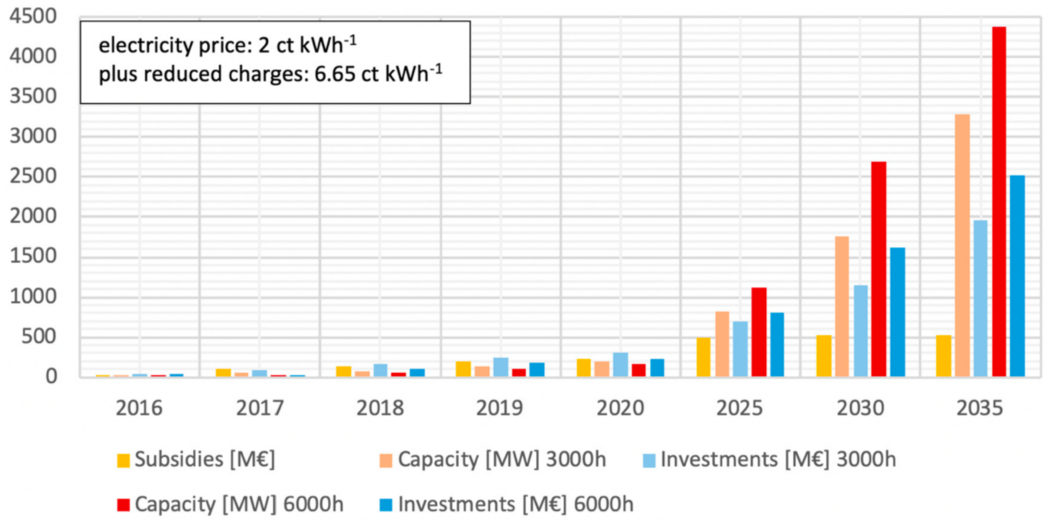

Figure 4.4: Simulation results for a progressive scenario with strict regulation adjustments and high initial subsidization. Accumulated capacities and investments are separately investigated for plant operation at 3,000 and 6,000 full load hours. The strong growth of capacity and private investments indicates adequate framing conditions for a successful implementation into the German energy system.

The vast capacity growth rate enables a significant capital cost degression, whereas successively enhanced GHG reduction quotas for enterprises enforce higher demands for PtF products. The individual measures introduce self-reinforcing effects, triggering the development of an electrolytic hydrogen and synthetic fuel economy. Also the fundamental impact of a powerful subsidization strategy can be derived from the results. The huge funding volumes realized until 2025 enable follow-up investments into new PtF projects as high as 2.5 billion euros until 2035. Consequently, the ratio of public funding and private investments exceeds 1:3 by 2030 and can nearly reach 1:5 by 2035. Interestingly enough, a comparable ratio target was published recently with a stated goal of 33 billion euros of investments for PtF projects out of 8 billion euros of funding [115].

Nevertheless, the latter values are significantly higher than those of the model results. The same applies to the simulated PtF capacities until 2035, which are considerably below the expected demand in most famous scenarios. Both deviations originate, however, from the initial purpose of the model: identifying *ways out of the niche into the market*. Once economically competitive, market mechanisms apart from those implemented into the model occur and exceed the model's framing conditions. By this means, further supply and demand mechanisms in an economically feasible environment arise, which are out of the scope of the model purpose and thus just not implemented.

In contrast to the findings for a successful integration of PtF concepts into the German energy markets, socio-economic consequences of their large-scale implementation are investigated within the follow-up publication of Chapter IX. Besides the calculated production costs of PtF products from Chapter VII and Chapter VIII, further data for a time horizon between 2020-2050 is aggregated from the literature and compared to scenarios for conventional fuel price developments. The significant price gap is displayed in Figure 4.5.

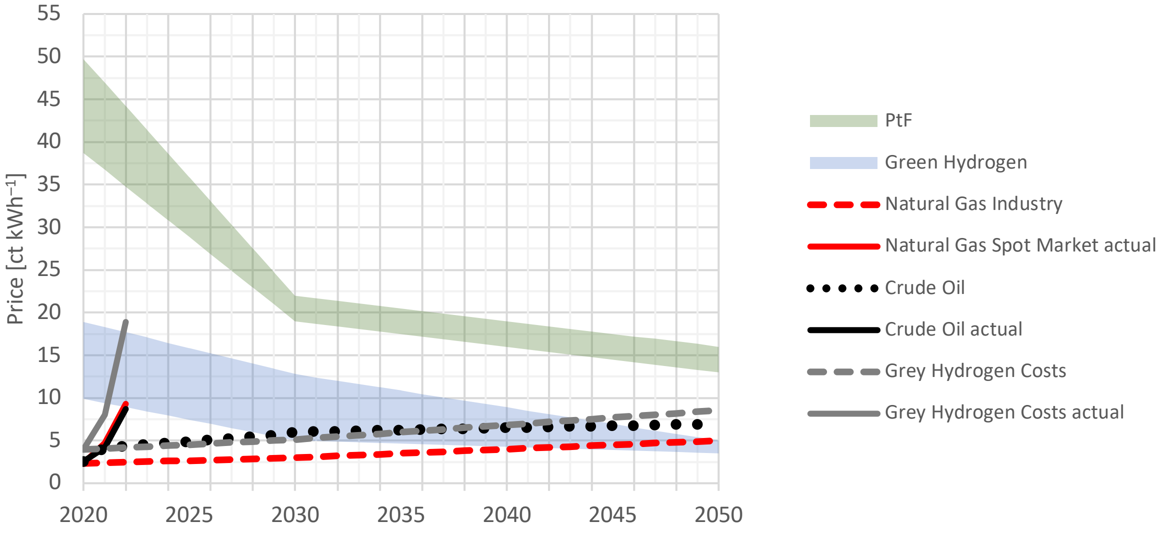

Figure 4.5: Projected price gap development until 2050 and actual prices of natural gas and crude oil until March 2022.

A rapid implementation of PtF products would provoke rigorous financial burdens for private and commercial customers with subsequent disruptive consequences for society and the economy. Impacts of such sudden price surges are experienced today as fossil energy carrier prices promptly increased to new all-time highs in the light of geopolitical tensions. Driven by energy prices, inflation rates drastically increased, supply chains are disrupted, and the purchasing power of customers decreases.

On the other hand, fossil fuels are considered too low-priced in the light of environmental damage compensation, as the combustion of fossil fuels entails high downstream costs (environmental impact costs). In Chapter IX, it is concluded that the energy mix of 2019 caused 156 billion euros of environmental impact costs, which are not compensated and will evoke a high burden for societies in the future. Thus, in the long term, the low energy costs of the recent past will have to be compensated by expenses for climate change-related damages.

Consequently, an adequate benchmark price for petrol, natural gas, and grey hydrogen (from steam methane reforming) was calculated based on energy price levels of 2020, including the respective environmental impact costs (Table 4.1).

Table 4.1: Specific CO_2 equivalents of all considered energy carriers and calculated benchmark prices for conventional fuels (cf. Chapter IX).

Energy carrier	**Specific CO_2 equivalents** g kWh^{-1}	**Benchmark price** ct_{2020} kWh^{-1}	**Price in 2020** ct_{2020} kWh^{-1}
Grey hydrogen	403	12	4
Green hydrogen	26	-	-
Natural gas	200	6.3	2.34
Petrol	275	9.9	4.7
Synthetic fuels	54	-	-

While the calculated benchmark price is up to 300 % above actual expenditures in 2020, a tradeoff strategy needs to be identified to prevent enormous climate change related societal costs in the long-term and to protect the economy from short-term energy price-related disruptions.

In public perception, the role of renewable energies has experienced a change lately. While the German *Energiewende* was steadily accompanied by scandalizing debates due to increasing electricity costs, renewable energy is suddenly acknowledged as an opportunity for energy independence and better price stability. In fact, the analysis in Chapter IX shows that the debates on electricity price developments were rather emotionally driven in the recent past, while energy price statistics reveal a stable and rather declining average electricity price for households from 2013-2020 in real terms. In addition, the average gross income increased simultaneously.

Nevertheless, compared to energy price levels of the past decade, renewable fuels such as electrolytic hydrogen and synthetic fuels will only be available at high costs in the short- and medium-term and thus foster energy price increases. However, a successive implementation is expected to feature gradual price increases instead of abrupt price jumps. Compared to energy price dynamics of the last decades back till the 1950s, such gradual increases are considered rather moderate. In addition, according to the findings in Chapter IX electrolytic hydrogen will become the cheapest energy carrier in comparison to crude oil-based products and natural gas in the long term. Hence, for a rapid implementation, policymakers need to develop strategies to incentivize the production and utilization of electrolytic hydrogen and synthetic fuels for industries and relief private customers concurrently.

Chapter V

5. Conclusion and Outlook

This work emphasizes both, the requirement of a large-scale PtF integration into the German energy system to contribute to the United Nations SDGs and climate mitigation, but also the necessity of integrated socio-techno-economic considerations for a reasonable PtF rollout. In this Chapter, an integrated discussion of the major results from all investigations covered by this dissertation is carried out. In Subchapter 5.2, the work is recapitulated with a focus on remaining research gaps and suggestions for future complementary research.

5.1 Conclusion

“In general, studies from well renowned research institutes see PtX as a major component in future energy systems. This is especially related to the potential provision of system services, e.g. chemical long-term storage of electricity and electricity-based synthetic fuel production, as well as balancing fluctuating renewable energy supply. Alternatively, an “all-electric” world is not a reasonable scenario and, as stated in Chapter 4, CCS technologies are not considered sustainable and face serious acceptance problems. However, most of the studies do not consider possible limitations of PtX concepts to fulfill the requirements.” These introducing words of Chapter VI’s Conclusion Section embed the topic of this work into the state of the art of PtF energy system integration knowledge. The system innovation of PtF concepts can be considered complex and systematic, as it interferes with and is exposed to a variety of technical, societal, economic, and ecological aspects. In consequence, comprehensive (holistic) analyses of the potentials and limitations of these concepts also require a multi-disciplinary character.

High capital and operating expenses appear to be the most limiting factors hindering a rapid diffusion of PtF concepts. The challenges of a dynamic operation of hydrocarbon synthesis for a reduction of hydrogen storage expenditures are discussed in Chapter VI. Process control complexity drastically increases, and catalysts of high thermal stability, e.g. platinum group metals, are required. Another important factor limiting applicable PtF capacities is the availability of renewable energy. The RE share within the German energy mix is still too low to legitimate immediate large-scale PtF capacities.

Nevertheless, industrial-scale plants are also topically important regarding proof of concept and capital cost reduction achievement. On a time-scale, electrolytic hydrogen production for either direct application in the mobility sector (e.g. heavy-duty transport) or industrial processes (e.g. steel and chemical industry) appears to be the first application of PtF concepts. Additionally, due to the direct link to the electricity sector, water electrolysis is frequently discussed as an opportunity for grid balancing services, direct utilization and storage of volatile wind and PV power. The investigation in Chapter VII reveals in this context that realizable RE utilization rates, hydrogen production efficiency and production costs are strongly dependent on the actual shapes of RE production patterns and the electrolyzers' ability to cope with them. Higher utilization rates can generally be achieved by PEMEL technology. However, (simulated) efficiencies of AEL are higher and partly overcompensate the lower utilization rates in terms of hydrogen production volumes.

Regarding economics, lower utilization rates are found to be potentially attractive due to longer stack lifetimes and correlated lower stack overhaul costs. Net production costs were evaluated at a minimum of 4.33 Eur kg_{H2}^{-1} for direct application of electricity generated from “old” onshore wind farms whose fixed EEG remuneration has expired, and up to 12.38 Eur kg_{H2}^{-1} for direct offshore wind power utilization with respective EEG remuneration. Nevertheless, a significant cost reduction for offshore wind power is expected.

For a more competitive electrolytic hydrogen and subsequent synthetic fuel production, a variety of aspects is required. On the one hand, the already above-mentioned CAPEX reduction is of high importance, but directly related to global capacity development due to economy-of-scale effects. Large capacities, on the other hand, will only be realized at more attractive economic framing conditions. The results of Chapter VIII reveal that consequent GHG emission restrictions are required to induce demand for PtF products. While an ambitious start-up subsidization accelerates capacity growth in the early years and enables faster CAPEX reduction and technology improvement, further single policy adjustments such as higher EU ETS prices or EEG fee exemptions are insufficient. They need to be supplemented by GHG emission reduction quotas for commercial customers. Improved framing conditions lead to a vast capacity growth within the simulations, while NPC's below 13 ct kWh^{-1} for any type of PtF product are hard to reach.

Although conventional energy carriers surged in price recently, the renewable substitutes from PtF processes will only be available at even higher costs, at least in the short term. However, from a societal point of view, the higher expenses for PtF fuels should be considered feasible. While their implementation could result in additional national energy costs of 10-100 billion euros a^{-1}, environmental impact costs from German GHG emissions in 2019 are stated as high as 156 billion euros. Besides economic and sustainability aspects, a phase-out of fossil energy carriers can be considered a chance for more geopolitical independence. Still, complete substitution of fossil energy requires a vast multiplication of renewable energy facilities not only in Germany, but worldwide. Nevertheless, as one of the leading GHG emitting countries, Germany should intensify all efforts toward a GHG neutral energy system. As discussed in this work, PtF concepts will play a key role in this way.

5.2 Outlook

The developed simulation models in this work are essential tools for the conducted analyses and provide solid results that are backed by validation approaches. Both models can contribute to further research beyond this dissertation. The LT electrolysis model is suitable for detailed techno-economic analyses considering very precise technological characteristics and constraints. However, further improvements can be implemented. As such, operating mode-specific electrochemical cell degradation effects would provide deeper insights into technical capabilities and favorable operating strategies. Also, the techno-economic analysis could be further improved with regard to resulting maintenance costs. Another point is the availability of electricity feed-in data. The applied data provides a resolution of 10-15 minutes per data point, although the model would allow for significantly higher resolutions. Especially in times of very dynamic electricity generation and respective electrolyzer operation, input data of better quality could give further insights into potential technology restrictions.

The ABM provides insights into dynamic market developments for a time horizon until 2035. As stated above, the central model purpose is the evaluation of an economic uptake of PtF concepts. Advanced market mechanisms reflecting the economic competitiveness of PtF, however, are not implemented. For further investigations, this could be an interesting add-on in combination with a longer time frame until 2050. Accordingly, the model could allow for an identification of conditions to achieve PtF capacity values as suggested in prominent scenarios which are in line with the *Paris Agreement* climate protection target. Nevertheless, the current model versions supply a reasonable starting point for such extensions and can be applied to gain further energy system transition knowledge for a more sustainable, climate-friendly future.

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Chapter VI

6. Socio-Technical-Economic Assessment of Power-to-X: Potentials and Limitations for an Integration into the German Energy System

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Socio-technical-economic assessment of power-to-X: Potentials and limitations for an integration into the German energy system

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ABSTRACT

The German Energiewende is facing new challenges with increasing shares of fluctuating renewable energies. Slow electricity grid extensions, restrictions in public perception as well as limited transformation progress in other sectors beside electricity cause major drawbacks in greenhouse gas mitigation. Power-to-X (PtX) technologies may be the missing link for a more resilient energy transition and provide both, renewable substitutes for fossil fuels as well as electricity grid balancing services owing to flexible operation and long-term storage abilities. Different PtX concepts proved operability in several worldwide distributed pilot projects. However, little is known yet about potential technical, monetary, societal and resource related scale-up limitations. In this paper, implications of these aspects for a large-scale energy system implementation are shown. From a technical perspective the concept of long-term flexible PtX operation modes is generally feasible and could become key for a more resilient future energy supply. However, economics are still the bottleneck for an extensive diffusion: in two scenarios for 2050 PtX may cause additional national annual energy costs between approx. 10 and 100 billion euros compared to an ongoing fossil fuel supply at current price conditions. Nevertheless, such expenses can be considered as reasonable in contrast to expenses for the compensation of climate change consequences of a future fossil fuel-based energy system.

1. Introduction

The energy transition in general and Germany's Energiewende in particular is based on an increasing contribution of renewable energy such as wind and solar power. Besides limited bio energy potentials, renewable electricity will be the only renewable energy source which may be utilized in all energy sectors [1]. As photovoltaic and wind power have the largest generation potential, but are highly fluctuating, there will be an increasing demand of energy storage in the long run [2]. Furthermore, to fulfill the international climate target of the Paris agreement (COP21), a limitation of global warming well below 2 °C above pre-industrial levels, greenhouse gas mitigation has to be achieved in other energy intensive sectors beside electricity as well. The electrification approach has limits, however: the globally growing aviation business as well as shipping and heavy road transport can hardly be electrified due to low volumetric energy densities of batteries [3,4]. Furthermore, industrial processes will continuously depend on hydrogen and hydrocarbon based raw materials.

Power-to-X (PtX) concepts, i.e. the conversion of renewable electricity into gases, fuels and chemicals, are considered as a major component in future energy systems [5,6]. For longer term storage, high volumetric energy density is an important issue, and this can be considered as the most prominent driving force for the development of these hydrogen based technologies [7]. All chemical PtX concepts are based on catalytic processes: Power-to-Hydrogen (PtH_2) is realized by electrolysis, i.e. electrocatalytic water splitting, which can provide hydrogen for Power-to-Methane (PtM), based on the Sabatier reaction, and Power-to-Liquid (PtL), based on either methanol synthesis or Fischer-Tropsch synthesis [8–10]. While the latter two synthesis routes are already well-established industrial processes operated at large scales, the two Power-to-Gas concepts are still subject to development and currently implemented as locally distributed applications at smaller

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Abbreviations: AE, alkaline electrolysis; CAPex, capital expenditures; CCS, carbon capture and storage; FTS, Fischer-Tropsch synthesis; PEME, polymer exchange membrane electrolysis; PtH2, Power-to-Hydrogen; PtM, Power-to-Methane; PtL, Power-to-liquid; PtX, pPower-to-X; RE, renewable energy; SOE, solid oxide electrolysis; SMR, steam methane reforming; TRL, technology readiness level

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scale. Within this paper, all prior introduced PtX concepts are analyzed except Power-to-Methanol. This is due to the current debate in Germany, which focuses on electricity based synthetic hydrogen, methane and Fischer-Tropsch drop-in fuels as substitutes for conventional fuels [11].

In the course of the Energiewende, PtX utilization is motivated from different perspectives. On the one hand, fluctuations in electricity production must be balanced by dynamic conversion and storage processes to limit the necessity of expensive grid expansions, or the alternative: the curtailment of production. Having this in mind, the import of PtX products as an alternative to a national production can be relativized to some extent.

On the other hand, PtX plants of high capacities would allow for a significantly increased renewable fuel supply in all energy sectors. Hence, PtX can contribute to an advanced supply security, i.e. to a more resilient energy supply. It provides several characteristics which are assigned as *design elements* of resilient energy systems, e.g. provision of storages, buffers, diversity and redundancy [12,13]. By this means, the conversion of electricity into chemical energy will amplify the utilization of storage facilities. Furthermore, a diversification of energy resources is realized with the production of both, electricity based synthetic gases and liquid fuels. All energy carriers enable redundancies in the energy system in terms of transportation and distribution infrastructures. The fulfillment of the design elements may keep the energy system rather flexible and enable the ability to better adapt and improvise in times of unexpectable disturbing events. Thus, PtX concepts could contribute to the resilience of energy systems, enabling both, a high supply security and climate compatibility. However, PtX technologies suffer from relatively low efficiencies along the process chains. Thus, a direct utilization of hydrogen might be beneficial compared to hydrocarbon production. Nevertheless, the direct use of hydrogen, e. g. in the transportation sector, is combined with several disadvantages regarding the permeability of tanks, the ratio of volume to energy content and the necessity for a completely new infrastructure.

With the assumption of all mentioned PtX concepts being essential for a resilient energy system transformation, we evaluated potential bottlenecks and barriers for the diffusion of PtX concepts in Germany. Clustered in three sections, critical aspects were addressed from a social, a technical, and an economic perspective. Within the subsections of Chapter 2 we will focus on technical aspects such as dynamic operation potentials and scale-up limitations of small-scale demonstration approaches with low technology readiness levels (TRL) as well as raw material availability with regard to a large-scale implementation, i.e. extensive diffusion of PtX concepts. Profitability and potential acceptance issues of centralized and decentralized PtX concepts will be addressed in Chapters 3 and 4. In Chapter 5, potentials for a large-scale energy system integration of PtX and contributions to a more resilient energy transition will be discussed, followed by a conclusion in Chapter 6.

2. Assessment of required system performances and potential technical limitations

The increasing share of renewables in the German energy system requires new flexibility options. Figures from the Federal Network Agency show that *surplus energy* from renewables recently rose to a significant level with 3.74 TWh being curtailed in 2016 and 5.52 TWh in 2017 [14,15]. *Surplus energy* in this context describes energy that cannot be fed into the transmission grid due to grid congestions resulting in wind and solar generators to be shut down. Thus, this curtailed energy was actually missing in the renewable energy balance and in fact, it was not a real surplus since the electricity demand in Germany can only be covered by nearly 100% renewable energy in very rare occasions. The transmission and distribution of renewable electricity to consumers is thus a major problem in times of high production rates. With electrolyzers as controllable electricity consumers such developments could possibly be minimized if located near grid congestion hotspots. Hence, a major criteria for the implementation of PtX concepts is going to be their location.

For a large-scale fuel production, however, the utilization of fluctuating surplus energy will be considerably insufficient. Thus, besides such decentralized concepts for the electricity sector, PtX installations of high capacities will be essential for renewable fuel and base chemical production, as could be implemented e.g. at refineries. Here, a high production rate will be favorable, whereas a dynamic operation capability is of less importance. With regard to the different technical requirements for both, centralized and decentralized concepts, the two Power-to-Gas processes (PtH_2 and PtM) and the Fischer-Tropsch synthesis as an example for PtL concepts were evaluated according to three major questions:

- Is it feasible to operate catalytic PtX processes in dynamic operation for an extended period, adapted to fluctuating renewable energy supply? What impact does the dynamic operation have on life-time of PtX plants and catalyst degradation?
- Is a scale-up of PtX processes into multi-MW scale feasible in the short-to-medium term? What are potential bottlenecks?
- Is there any shortage expected in raw material supply, especially with respect to catalyst precursors? Are there limitations in CO_2 and water availability?

Within the next subsections these questions will be addressed separately to low-temperature and high-temperature electrolysis concepts as well as the Sabatier process and the Fischer-Tropsch synthesis.

2.1. Power-to-Hydrogen via water electrolysis

The expected demand of installed electrolysis power depends on the chosen scenario. For an 85% reduction of CO_2 emissions (1990 to 2050) about 5 GW of power will be required from the year 2025 on, with a steep rise up to 15 GW not before the year 2033. In 2050, however, more than 70 GW will be installed according to a prominent study by Henning and Palzer. In addition, there will be a requirement of 20 GW electrolysis power for methanation and 5 GW for production of electricity based synthetic fuels, leading to a total electrolysis power demand of nearly 100 GW. This total demand of installed electrolysis power increases up to 200 GW when considering a 90% reduction scenario instead of 85% [2]. Assumptions on electrolysis capacity demand strongly vary in a broad selection of energy transition scenarios, depending if calculations are based on more or less ambitious climate protection targets and focused energy transition pathways. In this study, however, our calculations are based on the 85% and 90% reduction scenarios of Henning and Palzer.

Plant technology for such a scenario is already available. In particular, alkaline electrolyzers are realized in multi MW scale, even though electrolysis covers only 4% of the worldwide hydrogen demand [16]. A large-scale plant, which employs conventional alkaline electrolysis, was already realized in 1970 with plant capacity of 33,000 $m^3 h^{-1}$ (H_2 atm.) [17]. This equals installed electric power of 165 MW when considering an energy demand of 5 kW h/$m^3{}_{H2}$. From this it can be concluded that the energy of a park of 80 wind mills could already be successfully converted and stored chemically.

Another factor for hydrogen production is water availability. Eight liters of water are required for the conversion of 1 kg of hydrogen in theory. In reality, especially due to losses in water purification, 15 liters of water demand can be assumed for each produced kilogram of hydrogen or 0.45 l per kWh_{H2} [18]. By this means, 450 million liters or 450,000 m^3 of water will be needed per TWh of produced hydrogen. Annual total water demand in Germany is valued at 25.1 billion m^3, whereas the potential water supply is as high as 188 billion m^3 [19]. Thus, water demand can be considered as rather uncritical.

New developments such as high temperature electrolysis (solid oxide electrolysis, SOE), which allow for supplying part of the reaction enthalpy as heat, promise remarkable improvements of voltage efficiency (20% and above) compared to alkaline cell technology [20]. The technology profits from external input of heat that might be provided by subsequent exothermal processes (e.g. Sabatier or Fischer-Tropsch) leading to a high degree of heat integration. Its limitation, however, is the relatively low temperature level of both Sabatier and Fischer-Tropsch reactions. Further, due to the need of high operation temperature, this concept might come up with a sealing problem and severe material degradation; especially long-term stability of insulation and joining material is an issue [21]. Nevertheless, SOE is currently the most promising concept in terms of energy efficiency if heat integration is possible.

There is an ongoing debate on the risks and need of high-pressure operation of polymer electrolyte membrane electrolysis (PEME). Advantages are the possible absence of a hydrogen compressor as well as a reduction of energy consumption for compression and a reduction of overvoltage. Disadvantages, on the contrary, are a reduction of current efficiency, an increase of equilibrium potential difference, reduced life time of stack components due to hydrogen corrosion, higher investment costs and electrolyzer safety problems [22–24]. Being operated without high pressure, this technology is considered to be safe due to high product purity. When being operated at high pressure, however, there is a risk of getting mixed product gases even beyond explosive limits ("oxyhydrogen"). In order to stay clearly below the lower explosive limit, the challenge is to keep both product streams, hydrogen and oxygen, separate. The mixing risk depends on the level of the selectivity and permeability trade-off. The higher the selectivity for ion electromigration, the lower the undesired gas permeation becomes. This is, on the other hand, for the cost of relatively low ion permeability and, hence, higher internal resistance. For alkaline electrolysis (AE), which uses a diaphragm with a certain permeability for the gaseous products, the mixing risk is even more pronounced. Hence small and medium applications of these two concepts are unlikely. For more widespread applications and especially for household use, eliminating the mixing risk is of severe importance. There have been new concepts suggested for more efficiently decoupling of both half-cell reactions [25].

Thermodynamically water and the products of water splitting, oxygen and hydrogen, are in equilibrium at a voltage of 1.23 V. Water splitting electrolyzers, however, require higher voltages for the reaction to proceed in order to overcome energetic losses. This overvoltage, i.e. the part of the voltage that exceeds 1.23 V, can be divided into anodic and cathodic overpotential, which both increase with process intensity (current density) and activation energy and, thus, decrease with effectivity of the electrocatalyst used. For both part reactions, platinum alloys are currently best performers. Hence, the availability of sufficient amounts of platinum alloys could be a bottleneck [26]. While platinum is the catalyst of choice for the cathodes, it is ruthenium (and also iridium oxide) that can outperform platinum at anodes. With a demand of about 0.5 mg cm^{-2} at a cathode of polymer membrane based electrolyzers [24], this gives, when considering a power density of 5 W cm^{-2} [27], a total demand of 10 t[1] for the "100 GW power scenario". Such an amount equals 4.6% of the global platinum use that totaled 218 t in 2015 [28]. Projected demand estimates for platinum in 2050, which did not consider the platinum demand of water electrolysis, range from 400 to 1200 t per year [29]. In comparison the global reserve (that part of the resources with a reasonable potential for becoming economically available resources) is estimated at 69,000 tons of platinum-group metals [30]. This emphasizes the need for high research efforts to replace platinum alloys by inexpensive and abundant elements such as nickel and iron.

With respect to the fluctuation of renewable energies, surprisingly little is reported in literature about the sensitivity of water electrolysis on unstable electric power supply conditions. This is an issue of highest importance as renewable energies such as wind and solar naturally fluctuate. It is known that PEME can be operated in the total partial-load range, whereas AE is limited to 20–100 % of its nominal load [22]. Furthermore, high pressure operation conditions (more than 10 bar) cause a deterioration of partial load behavior [31]. Anyhow, a more profound analysis of long term behavior under flexible load cycles has to be part of future research activities. A nickel based catalyst, for instance, as it is used in conventional anodes for alkaline water electrolysis, is stable in steady electrolysis, but it corrodes easily with potential cycling [32]. Further energy demand may rise under fluctuating conditions [33]. Another issue related to dynamic electric power supply is fluctuating temperatures within the catalytic layer causing thermo-mechanical stress. This can damage or even destroy the catalyst and is known - for catalytically coated supports - as a reason for short life times [34].

Table 1 provides an overview of relevant criteria's for three discussed types of electrolyzers. It can be concluded, that plant technology is generally available for an extensive implementation into energy systems. However, each technology exhibits at least one constraint and that is a limited potential for dynamic operation control for AE and SOE. For PEME platinum group metals are required, which can be considered as critical resources and especially may face high expenses if the worldwide demand considerably increases.

2.2. Power-to-Methane via Sabatier reaction

The Sabatier reaction produces methane that can be considered as "*green SNG*" when "green hydrogen" and a sustainable carbon source is being used. Even though *green SNG* cannot be as cost efficient as hydrogen, it shows lower self-discharge in long term storage. The required carbon dioxide can be obtained by carbon capture from flue gas of fossil-fired power plants, e.g. via absorption (carbon scrubbing) for the cost of a high energy penalty of at least 16.3% of additional energy input [35,80]. However, the utilization of fossil-based CO_2 for electricity based synthetic fuel production enables a recycling, but does not prevent greenhouse gas emissions as long as the fuel is finally combusted again. Instead, pure CO_2 is available from biomass combustion, biogas upgrading and biofuel production with concentrations of 3–8 vol.-%, 40 vol.-% and up to 100 vol.-% respectively [35,78,79]. According to a recent study about 17 million tons of biogenic CO_2 could annually be available in Germany. This number refers to large-scaled sources (biogas-upgrading and solid biomass CHP plants larger than 1 MW_{el}) with a reasonable exploitation potential [36].

The actual CO_2 demand for PtX processes depends on the chosen scenario. Klaus et al. calculated 55 TW h of yearly methane demand until 2050. Based on the molecular weights of CO_2 and methane and related to the energy content of methane, 0.2 tons of CO_2 are required to produce 1 MW h of methane. Thus, the demand for 55 TW h will be 11 million tons of CO_2 [37]. However, biogenic CO_2 will very unlikely cover the entire carbon demand for the total electricity based synthetic fuel production due to limited sustainability potentials.

Without sufficiently high amounts of biomass, carbon dioxide needs to be recovered from air. Any kind of process requires, due to the low concentration of CO_2 in air, a throughput of 3 million cubic meters of air per ton of CO_2 recovered and even much higher amounts of energy compared to carbon capture from flue gas [38]. According to LBST, 1 ton of CO_2 from air requires 1.9 MWh_{el}, if absorption/electrodialysis technology is applied [36]. Another air capture technology was invented by the ETH Zurich spinoff Climeworks. The technology is based on an adsorption/desorption cycle, which allows to supply the major energy share in terms of low temperature heat (95 °C). The actual energy demand corresponds to 1.5–2.0 MWh_{th} and 0.2-0.3 MWh_{el}.

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[1] 0.1 mg/W = 0.1 t/GW

Table 1
Overview of major criteria's for the evaluation of integration potentials for electrolyzers into energy systems. The three types are compared with concern to state of the art, scaling potentials, resources and their potential for flexible operation modes for grid balancing services [27,84,98].

Criteria	Alkaline Electrolysis	Protone Exchange Membrane Electrolysis	Solid Oxide Elektrolysis
State of the art	– Technology readiness level (TRL): 9 – Industrial application, e.g. Assuan – Capacity: 33,000 Nm^3 H_2 → 165 MW (assumption: 5 kWh m^{-3})	– TRL: 8 – Pilot projects in multi MW scale – e.g. Energiepark Mainz, 6 MW	– TRL: 5-6 – Pilot projects in multi kW scale – e.g. Salzgitter Steelworks, 150 kW
Scaling potential	– Uncritically – Large scale operation	– Uncritically – Up-Scaling in progress	– Uncritically – 20 MW plant expected in 2020
Resources	– Uncritically – Nickel catalysts	– Critical: Platinum & Iridium – Platinum group metal reserves: 66,000 t → Assumption for 10 GW: 1 t Pt → 0.5 % of worldwide demand in 2014	– Uncritically – Nickel and Ceramics catalysts
Potential for dynamic operation	– Critical – Ni-catalysts easily corrode – Load range: 20 – 100 %	– Uncritically – Catalysts remain stable – Suitable for flexible operation – Load range: < 10 – 200 %	– Critical – High thermal stresses → critical long term stability – Load range: < 50 – 100 %
Preferable application	– Preferably constant operation – Limited capability of grid balancing services – (Centralized) large scale plants	– High security – High capability of grid balancing services – (Decentralized) small to medium scale	– Suitable for sites with waste heat resources – Limited capability of grid balancing services – (Centralized) large scale plants

For an 85% reduction of CO_2 emissions (based on energy conversion) about 3 GW of installed methanation power will be required not before the year 2030. This equals 500 plants of the 6 MW type installed by Audi AG in Werlte, Germany. A steep rise, however, is expected from 2045 on, exceeding 20 GW in 2050 [2].

Today the production of „green SNG" from renewable energies in small, distributed (pilot) plants requires relatively large buffer tanks. Their volume could be reduced by dynamic production, which is technically feasible in the range of 50–100 % of a plants nominal load [39]. However changing gas loads could reduce catalyst lifetime mechanically due to thermal stress especially at the hot spot. Further a faster deactivation of the catalyst is possible. A more dynamic operation can be expected when using monolithic sponges with improved heat transport by conduction allowing for better hot spot control.

The state of the art catalyst for Sabatier reaction is nickel which provides high methane selectivity and relatively high yield. Ruthenium, however, is even more active: for a single tube reactor with a turnover rate of 1.7 kg/(m^2*s) the necessary catalyst load is 3.5 g ruthenium to convert 12 kW.[2] From this it can be estimated that, for a capacity demand of 20 GW in 2050, 5.8 tons of ruthenium will be required in total. This equals about 0.01% of the world's global reserve of platinum-group metals and nearly 45% of US ruthenium imports in 2017 [30].

When using nickel instead, its comparatively lower activity requires higher temperatures for obtaining the same reaction rate. This in turn restricts the yield of the reaction even at multi-stage operation with intermediate cooling. It is due to the thermodynamics of exothermal reactions - such as Sabatier reaction – that reactions yield decreases non-linearly with increasing temperature. Recently it was shown that cobalt, an element almost as well-available as nickel, performs much better in this respect: If particle size of cobalt coating is properly chosen, a temperature of 300 °C is sufficient for a reasonable turnover frequency [40], for which nickel requires higher temperatures. However, this needs to be confirmed at large-scale.

Assuming that the activity of nickel is one tenth of the activity of ruthenium, about 60 tons of nickel will be required to realize a methanation capacity of 20 GW. Since this is no more than 0.003% of the actual global mine production capacity per year [41], there is no limitation to be expected with respect to raw material supply for the production of Sabatier reactors.

Given a limited yield of about 85%, the Sabatier reaction provides a product with a concentration of carbon dioxide and hydrogen which is too high for many applications. Subsequent purification by state of the art treatment processes, such as absorption, adsorption or membrane separation is expensive and reduces the overall process energy efficiency. Therefore, all efforts in further process development should aim at improved highly-performing, low-cost catalysts to allow for highest yield conversions. The higher the activity, the shorter the reactor length required for that high yield. Thus, depending on the activity, capital expenses of the methanation process will be determined either by the price of steel (on top of engineering and instrumentation cost) at lower activity or by peripheral equipment and engineering alone.

2.3. Power-to-Liquid via Fischer-Tropsch synthesis

Fischer-Tropsch synthesis (FTS) is a much more complex reaction compared to Sabatier reaction as it converts carbon monoxide and hydrogen into a mixture of gaseous and liquid hydrocarbons. This complexity is one reason for the current preference to operate FTS stationary at large-scale only. It is a process that has been applied for decades in coal liquefaction with production rates of low-sulfur diesel fuel in the order of magnitude of 1 million metric tons per year. First attempts for scaling down FTS-plants turned out to be challenging. Nevertheless, with the high heat removal capability of microreactor technology, single pass conversions of up to 75% have been realized [42]. Higher conversions are challenging as they lead to high concentrations of water that can result in reoxidation of the active cobalt catalyst.

Like Sabatier reaction, FTS is a strongly exothermal process requiring permanent cooling to prevent hot spots or even run-aways. In case of FTS cost and temperature is even more important, as the product composition is very sensitive on temperature changes. While Sabatier reaction produces methane only, the product in FTS comprises alkanes, alkenes, alcohols, and other oxygenated hydrocarbons. The increased process complexity causes a slower partial load behavior than known from the Sabatier reaction. However, dynamic partial load operation can be realized with a minimum of 50% of the nominal load and is therefore still in a feasible order of magnitude [39]. Subsequent to FTS, the product mixture is to be refined, similar to crude oil. Any changes in composition would increase downstream processing demand. All this makes dynamically operated small-scale plants challenging.

Expected power demand will be, according to the 85% CO_2-reduction scenario, about 2 GW, 4 GW and 5 GW in the years 2022, 2027, and 2030 respectively [2]. This demand can be considered in context with the performance of a large-scale production facility for transforming syngas into liquid, e.g. Pearl, Qatar [43]. Substitution of its production capacity (140,000 BPD) by means of electricity based FTS fuels would

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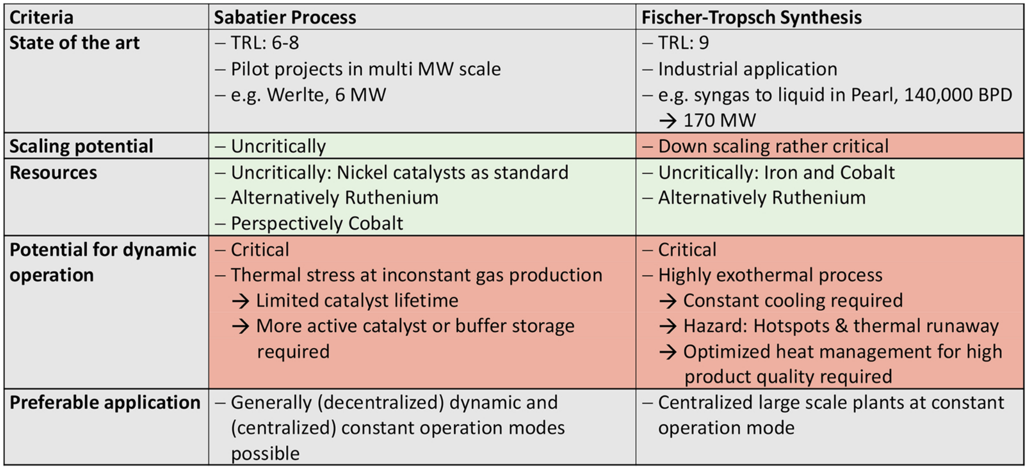
[2] Case study ($p0 = 10$ bar, $T0 = 300$ °C, $Da = 0.1$, $Se = 2.55$, $Y = 92\%$, $L = 0.5$ m, $D = 25$ mm) according to Kiewidt and Thöming [83]

Table 2
Overview on major criteria's for the production of hydrocarbons via PtG and PtL. Both discussed processes are compared regarding state of the art, scaling potentials, resources and their potential for flexible operation modes for grid balancing services [84,98].



Criteria	Sabatier Process	Fischer-Tropsch Synthesis
State of the art	– TRL: 6-8 – Pilot projects in multi MW scale – e.g. Werlte, 6 MW	– TRL: 9 – Industrial application – e.g. syngas to liquid in Pearl, 140,000 BPD → 170 MW
Scaling potential	– Uncritically	– Down scaling rather critical
Resources	– Uncritically: Nickel catalysts as standard – Alternatively Ruthenium – Perspectively Cobalt	– Uncritically: Iron and Cobalt – Alternatively Ruthenium
Potential for dynamic operation	– Critical – Thermal stress at inconstant gas production → Limited catalyst lifetime → More active catalyst or buffer storage required	– Critical – Highly exothermal process → Constant cooling required → Hazard: Hotspots & thermal runaway → Optimized heat management for high product quality required
Preferable application	– Generally (decentralized) dynamic and (centralized) constant operation modes possible	– Centralized large scale plants at constant operation mode

cause a power demand of about 18 GW,[3] which is already more than three times the predicted demand for 2030. CO_2 demand for the PtL process depends on the chain lenghts of produced hydrocarbons. Recent studies suggest 0.27-0.34 tons of CO_2 for 1 MW h of electricity based synthetic crude oil substitute [9,44]. In an extreme case scenario for a greenhouse gas neutral energy supply in Germany, 552 TW h of electricity based synthetic liquid fuels are projected for 2050, involving a CO_2 demand of 149–187.7 tons [45].

Currently the catalyst's elements, which are usually considered as most relevant for future applications, are Fe, Co, and Ru. While the latter two remain in the metallic state under the reducing conditions during operation, iron catalysts form a number of oxides and carbides during reaction. This necessitates control of these phase transformations in order to maintain catalytic activity. Availability of catalyst is not a limiting factor. For 5 GW the total mass of catalyst required is 200 t of active element.[4] In case of iron, the fourth most abundant element in Earth's crust, this amount is negligible. The same with cobalt (refined cobalt production 2015: 97,400 t per year) [46]. Ruthenium, on the other hand, is much too expensive to be used as main active component. However, even as minor component of about 1 wt.-% the amount required is still in the order of magnitude of 2 t, which is quite a lot when considering that the global consumption of ruthenium was 34.2 t in 2016 [47].

The active catalyst is obtained on stream. Iron, the most prominent Fischer-Tropsch catalyst, is not active by itself, even when being in the reduced state. It is rather an iron carbon compound which requires days or even weeks to be formed during operation. Thus, it takes a certain period of time to reach reasonable yield and selectivity. The other candidate is cobalt, which produces methane when carbon dioxide is used as feed and becomes highly Fischer-Tropsch active when carbon monoxide is used instead. Like iron, cobalt has to be reduced at hydrogen atmosphere before usage.

Both catalysts are based on abundant raw materials and can be produced by relatively simple precipitation processes. Recently it was found, however, that more sophisticated coating processes, such as sol-gel techniques, allowed for control thickness of catalyst layer as well as size of cobalt nanoparticles. By this means, the best compromise for reducibility and activity can be achieved [40].

In contrary to the raw materials of the catalysts, which are relatively cheap (in case of cobalt about 65,000 €/t) [48], steel required for piping and reactor tubes and vessels determines the plant cost. However, this has to be qualified since the cobalt price increased by 113% from 2016 to 2017 [48]. This is, inter alia, due to the rising demand for lithium-ion battery cathodes [49]. A continuation of this development might refute the initial statement.

Table 2 comprises the major technical evaluation results for both discussed hydrocarbon generation processes, Sabatier process and Fischer-Tropsch synthesis. For both processes it can be concluded that a dynamic operation control remains critical as long as catalysts with comparably low activity are applied. By this means hydrogen buffer tanks for constant process operation would be needed. However, there are research efforts for a small scale flexible process design of Fischer-Tropsch reactors [50].

3. Economic evaluation of centralized and decentralized PtX concepts

The results of the previous subsections show that both, large-scale (centralized) and small-scale (decentralized) concepts are generally realizable from a technical perspective. This sections focus is on the economic viability of such PtX approaches. The most prominent economic dilemma is given by the contradiction of a maximized PtX plants annual operation time and the provision of system services to minimize the curtailment of renewable energy. For a reduction of wind power down throttling, excess PtX capacity is required.

Repeatedly it is argued that a further improvement of voltage efficiency of the electrolysis could solve the economic problem. However, in a recent study it was shown that business cases can hardly occur even at high utilization rates of 6000 full load hours for centralized concepts and progressively assumed technical improvement. An agent-based model was developed to investigate business case evolvement and related capacity growth depending on several adjusted framing conditions. Based on stakeholder information, representative investor and customer groups for PtX were characterized and implemented as agents, which aim to sell and buy PtX products in the national energy markets. Related to their individual characteristics, the agents attempt to create business cases and/or purchase PtX products at specific price thresholds. Based on the development of demand and business cases in a defined time horizon, the resulting capacity growth could be

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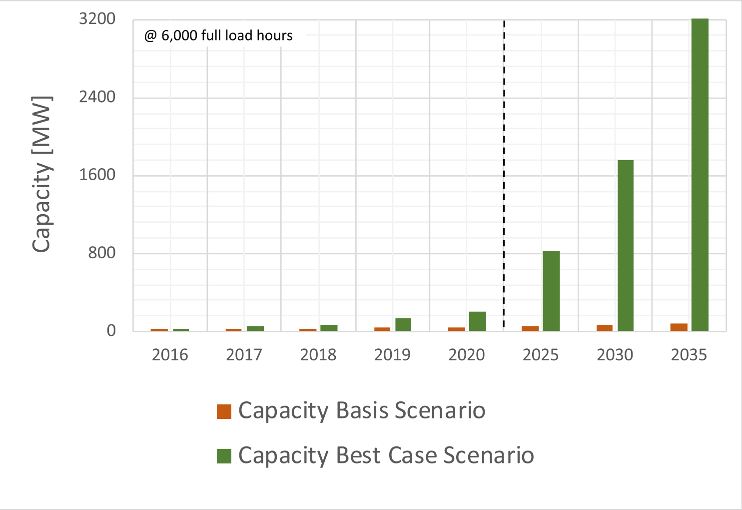
[3] Assumption: 1 barrel = 1,700 kWh; Conversion Efficiency: $\eta = 55\ \%$

[4] Given a typical space velocity of 0.1 mol synthesis gas per kg catalyst per second (catalyst: active elements, without weight of alumina support) Estimation: heat of combustion CH_4 = 880 kJ/mol and 0.03 mol CH_4/(kg s) gives 26 kJ/(kg s) = 26 kW/kg catalyst, which equals 80 t



Net market prices in Germany (2016)

Electricity:	2-3 ct kWh^{-1}
Gas:	1-3 ct kWh^{-1}
Petrol/Diesel:	4-7 ct kWh^{-1}
Biofuels:	7-8 ct kWh^{-1}
Hydrogen (SMR):	6-7 ct kWh^{-1}

	2035	
	CAPex [€ kW^{-1}]	Product [ct kWh^{-1}]
P2H$_2$	1,292	23.6
P2M	2,630	30.4
P2L	3,500	38.7

	2035	
	CAPex [€ kW^{-1}]	Product [ct kWh^{-1}]
P2H$_2$	520	12.8
P2M	1,000	15.4
P2L	1,000	15.4

Fig. 1. Simulation results for PtX capacity growth until 2035 and related production costs for hydrogen as well as electricity based synthetic methane and liquid fuels in two scenarios: In a *Basis Scenario* todays legal framing conditions remained unchanged throughout the model run. In a *Best Case Scenario*, framing conditions were optimized and allowed reduced production costs and capital costs as a result of scaling effects [51].

evaluated. With the adjustment of framing conditions in specific scenarios, the most important parameters for a successful diffusion of PtX were characterized. It was revealed that a high diffusion of electricity based synthetic fuel production rather requires consequent research funding and subsidies for the construction of new installations to enable capital expenditures (CAPex) reduction through scaling effects. Furthermore, strict greenhouse gas mitigation quotas for industries need to be implemented to achieve competitiveness to fossil fuels. In a best case scenario without surcharges for input electricity, production costs of 12.8 cent kWh^{-1} for hydrogen and above 15 cent kWh^{-1} for methane and liquid fuels were calculated [51], also see Fig. 1.

In addition, Henning and Palzer showed that for a total conversion of the energy system and for a nearly full wind energy usage (almost no down throttling), the demand of electrolysis plants will be about 100 GW of installed electric power. This in turn leads to operation times as low as 2,000 h per year and costs of about 18 ct kWh^{-1} of hydrogen. With reduction of installed power below 20 GW, however, the operation times improve slightly progressively, while the improvement of cost is disproportionally lower: For exceeding an operation time of 5,000 h per year the cost drop down to 13 ct $kWh^{-1}H_2$ only [2]. Table 3 comprises typical net price ranges for fossil fuels, electricity and hydrogen from steam methane reforming (SMR). At current legislation, input electricity for PtX processes is surcharged with high additional fees and taxes, if product X is not used for electricity generation.

Profitability is mainly dependent on investment costs, costs for input electricity, number of full load hours and revenues at appropriate markets. Whereas even centralized concepts with high utilization rates can hardly run economically, business cases might be even harder to create for decentralized PtX concepts with a low utilization in times of high electricity production only. Therefore, two different cases for decentralized concepts are compared:

- A PtX entity is directly connected to a renewable energy unit and converts surplus electricity into electricity based synthetic fuels.
- A PtX entity is directly connected to a renewable energy unit which was constructed for electricity based synthetic fuel production only and is not connected to the power grid.

In both cases the PtX entity may not be in the duty of compensating any fees for input electricity as it is disconnected to the public electricity grid. For the first case, the intended benefit for the energy system could be a reduced demand for power grid extensions. As grid extensions are expensive and much slower than RE expansion (e.g. due to lack of social acceptance, [52]), such a concept would be highly attractive: Surplus energy will be chemically stored and used in other sectors or reconverted to electricity in times of low wind and photovoltaic power. The above mentioned increasing curtailment of renewable electricity, which caused a financial damage of 610 million euros in 2017 and is leading to increasing network fees for consumers, might be balanced [15].

Table 3
Overview of fossil fuel net prices and hydrogen from steam methane reforming [87,90]; [93,96]. Input electricity for PtX processes is further surcharged by fees and taxes at current legislation in Germany [86,89]. Assumptions on investment costs are based on [92,21,85,91,94,95,97].

Energy carrier	Prices		Technology	CAPex
	€ kWh^{-1}	specified units		€ kW^{-1}
Natural gas	0.01-0.03	0.08-0.25 € Nm^{-3}	*Alkaline electrolysis*	800-1,500
Crude oil	0.05-0.07	85-119 € bbl^{-1}		
			Protone exchange membrane electrolysis	2,000-6,000
Bio fuels				
Gas	0.08	0.88 € Nm^{-3}	*Solid oxide electrolysis*	2,500-8,000
Diesel	0.08	0.83 € l^{-1}		
Petrol	0.07	0.68 € l^{-1}	*Methanation*	720
Hydrogen	0.06	0.21 € Nm^{-3}	*Fischer-Tropsch Synthesis*	1,000
Electricity	0.02-0.03			
- Surcharges for PtX entities in 2016	0.196			

The German Energy Agency expects limited feed-in of 80% for wind and 70% for photovoltaic installations of their theoretical peak power, since costs for power grid extensions would increase inversely proportional related to the additional energy yield [53]. Brunner et al. calculated resulting full load hours for the first case based on load profiles and the assumption of 4000 utilization hours of photovoltaic and 7000 utilization hours of onshore wind power and the reduced feed-in of 70% and 80% of the theoretical peak power. In accord, photovoltaic power would be curtailed 83 h per year and onshore wind power for 46 h per year. From this it was presumed that a resulting full load operation of below 100 h will eliminate profitability even at free input electricity and CO_2 because of too high CAPex. But even progressive investment cost reductions will not help to create business cases at low utilization rates. For hydrogen production costs of 1.76–6.11 € kWh_{H2}^{-1} were calculated, which is up to factor 100 higher than hydrogen from SMR according to Table 1 [54]. However, as stated in Chapter 2, dynamic PtX concepts require additional expenditures which were not considered in this calculation. Thus, the barrier for profitability will further increase. Electricity based synthetic methane production would end up even more expensive due to lower process efficiency and higher CAPex. The Fischer-Tropsch synthesis instead is not applicable for such low operating hours due to complex process control.

In the second case it is assumed that the renewable energy source was installed to serve PtX entities only. Thus, electricity costs need to be calculated as high as the production costs of the renewable source according to plant life-time. A direct connection to PtX plants exhibits several advantages. As the public power grid is not used, corresponding charges, fees and taxes do not need to be compensated. In accord to resilience such concepts are beneficial as well, since fuel and base chemical production becomes at least partly independent from power networks and possible shortages. In this case it requires optimized scaling of input power of the PtX installation and output power of the renewable energy source to grant high utilization rates. Thus, the PtX installation capacity should be significantly lower than the capacity of the RE plant.

Kost et al. calculated RE production costs of 4.5–10.9 ct kWh^{-1} for wind onshore and 8.0–14.0 ct kWh^{-1} for photovoltaic electricity, individually dependent on utilization and location. Future developments are estimated to range between 4.2–10.2 ct kWh^{-1} and 5.5–9.5 ct kWh^{-1} [55]. With regard to these assumptions it can be expected that business cases may arise, if CAPex degression for both, RE and PtX plants occur, combined with high utilization rates as well as increasing prices for fossil energy. However, high utilization rates require dynamic operation capability, leading to more extensive investment costs compared to power grid connected concepts.

4. Evaluation of potential limitations in social acceptance

The existing pilot projects in Germany did not experience problems concerning social acceptance [56]. Furthermore, direct utilization of hydrogen did not appear to be confronted with safety issues [57]. Instead of potential scandalization and limited acceptance, a few of these projects rather achieved support by a better willingness to pay of customers for the electricity based synthetic products. The motivation to support the development of PtX innovation is seen as a main driver for the higher willingness to pay. As stated above, the PtX concept is widely recognized as a future core element of the energy system transformation process. It allows for a shift of renewable electricity to other sectors and this way enables a “green” gas und fuel consumption for the first time without the use of biomass. In accord, it may be expected that especially decentralized small-scale PtX concepts for the utilization of excess electricity will not be confronted with scandalizing processes. Instead, communities aiming for a self-sustaining energy supply are aware that PtX may become a major component within local energy systems [12].

In general it is acknowledged that energy storage and conversion concepts are better accepted than infrastructural measures such as power grid extensions [31]. The latter is one of the major drawbacks in the German energy transition as nearby installations are often refused by activists. However, a consequence of slowed grid extensions are increasing curtailed excess electricity volumes. The compensations for RE plant operators in turn increase electricity prices, leading to new constraints for the Energiewende. Thus, energy storage and conversion concepts such as PtX may be the missing link to solve both, perception problems as well as lacked excess electricity utilization. Buenger et al. report that energy providers see PtX installations to compensate for bottlenecks in transmission networks. However, PtX may rather complement and not compensate grid extensions [58].

Experience with centralized large-scale PtX entities is not available. A look at previous technological innovation processes reveals that especially research and pilot projects are often better perceived than first attempts of large-scale implementations, e.g. in case of CCS (carbon capture and storage) projects [59]. CCS was formerly seen as a major innovation for reaching the greenhouse gas emission targets in many German economic optimization models. In consequence of serious scandalizing processes in public, however, CCS projects were barely ever realized in Germany [60].

However, such cohenrences are strongly dependent on situational factors. Sonnberger et al. recently stated impact factors having an effect on social acceptance for energy technologies. They found four key values determining acceptance: confidence in companies and/or actors, general attitude to the Energiewende, perceived fairness of the Energiewende, perceived benefit of the technology and perceived risks and disadvantages of the technology. Thus, citizens are willing to support transformation processes if they are convinced of the purpose. If this is the case people most likely will be willing to contribute [61].

The promotive support of well trusted research institutes as well as of prominent NGO’s may also indicate a high acceptance potential for PtX installations beyond pilot scales. Nevertheless, even though large-scale installations may not experience acceptance issues directly, the increasing demand for renewable electricity for electricity based synthetic fuel production may lead to indirect scandalizing processes. Depending on the chosen scenarios, a coverage of the total national fuel and base chemical demand may lead to increasing renewable energy capacities up to factor 15 compared to today’s share [45,62,63]. This is also because of high conversion losses which might further decrease acceptance for PtX processes. Today, critics of renewable energy, especially of wind power, argue with spoiled landscapes, hazards for endemic bird populations and harmful noise pollution. Another major argument is that, even though visible to a large extent, renewables contributed to a share of only 15% of the end energy consumption in 2015 [64]. So the source of expectable main objections against the development of PtX will not be in the conversion technologies themselves but in the enormous extension of wind energy, especially onshore.

However, according to recent surveys, 93% of the German population believe that the expansion of renewables is of exceptional importance. 62% stated to support new installations in their surrounding neighborhood. Thus, the “not in my backyard” phenomenon may only affect the extension of onshore wind energy plants. At least, a higher support of residents living close to renewable energy installations compared to others appears to be present [65,66].

With regard to the PtX concept an overall conclusion whether acceptance will remain high or decrease during an extensive energy system integration process is not possible. However, with a focus on the whole transformation process PtX may technically solve current critiques such as lacked excess electricity utilization and this way increase its perception. Nevertheless, a national and completely renewable fuel supply from German production will be very unlikely, limiting the national PtX capacities as well. Thus, the Federal Environment Agency suggests to import electricity based synthetic fuels to a large extent directly from abroad, where larger area potentials are available [67]. As

Table 4
Comparison of the demand for electricity, gas and liquid fuels and available storage capacities [88].

		Electricity	Gas	Liquid fuels
Demand	[TWh a^{-1}]	610	909	711
Average power	[GW]	70	100	80
Storage capacity	[TWh]	0,04	217	250
Share of renewable energies	%	˜ 36	˜ 1.5	˜ 6

already mentioned in the introduction this serves well for uncritical infrastructures and other services. However, from a resilience point of view a large scale national PtX diffusion would be favorable and could be supplemented by imports.

5. Contributions and restrictions to a resilient energy system transition

As stated above, an extensive implementation of PtX is beneficial in order to implement some design elements into energy systems. According to Table 4, there are large capacities for gas and liquid fuel storage available in Germany, whereas only a low capacity of pumped hydro storage for electricity generation is available. With PtX, the large storage capacities for methane and liquid fuels can remain sustained and contribute to a less vulnerable future energy supply.

Table 4 also indicates a comparably low share of renewables in gas and liquid fuel supply, i.e. in the heat, industry and mobility sectors. Nevertheless, as stated above, hydrocarbon-based fuels will also play a significant role in a future CO_2 neutral energy system. Today, this small share is provided via biofuels. However, due to land use conflicts, fuels generated via PtX are widely recognized as an advantageous alternative [68,69].

Within the previous sections it was revealed that PtX concepts are technically feasible, even for flexible operation modes and excess electricity utilization and thus have a high potential to contribute to a more resilient energy transition. However, several limiting factors, especially economic feasibility, may restrain the diffusion of PtX. In Section 3 it was pointed out that, even in a *best case scenario*, electricity based synthetic fuels will not be competitive to today's fuel prices. Thus, the substitution of fossil fuels may induce a much more expensive future fuel supply of above 12 ct kWh^{-1} for hydrogen and more than 15 ct kWh^{-1} for methane and liquid fuels, even if legal framing conditions are widely adjusted. This, however, may arouse societal problems and requires further consideration.

According to a prominent study from the Federal Environment Agency, the national fossil fuel consumption in all sectors was 895 TWh of natural gas and 696 TWh of liquid fuels in 2010 [70]. Based on the prospected electricity based synthetic fuel demand for 2050 in an extreme case scenario for a greenhouse gas neutral energy system [70] and calculations in Table 5, the annual national expenses for a renewable gas and liquid fuel supply via PtX could almost treble with up to 175.4 billion euros compared to 59.6 billion euros for fossil fuel supply at constant price conditions. However, in a more moderate scenario for a 85% greenhouse gas reduction until 2050 compared to 1990 from Henning and Palzer, the assigned PtX demand is considerably lower with only 29.4 TWh of methane and 27.3 TWh of liquid fuels [2]. Based on the production costs from Fig. 1, the annual costs for electricity based synthetic methane and liquid fuels would sum up to 8.7 billion euros in this scenario, respectively. Thus, the additional expenses for PtX are not only related to chosen technical transition pathways but also to the greenhouse gas reduction goals.

Nevertheless, according to a study from the German Institute for Economic Research, the expenses for the compensation of climate change consequences could sum up to 800 billion euros until 2050 and 3000 billion euros until 2100, if any further climate protection measures are applied [71]. This indicates that resilience efforts like a PtX implementation can still be considered generally economically worthwhile on the long scale, even though such a system will be much more expensive than the fossil-based system of today. The assumptions also correlate to findings of Burke et al. who investigated the negative impacts of global warming on the global economic output [99]. Furthermore, financial penalties for missed climate protection targets must not be neglected within this discussion. Following the current trend, Germany will not reach its climate protection targets for 2020 and 2030 and will have to financially compensate its excess emissions. According to Deutsch et al. up 60 billion euros of penalty expenses might occur for Germany until 2030 at the current trend [72].

6. Conclusion

In general, studies from well renowned research institutes see PtX as a major component in future energy systems. This is especially related to the potential provision of system services, e.g. chemical long term storage of electricity and electricity based synthetic fuel production as well as balancing fluctuating renewable energy supply. Alternatively, an "all electric" world is not a reasonable scenario and, as stated in Chapter 4, CCS technologies are not considered sustainable and face serious acceptance problems. However, most of the studies do not consider possible limitations of PtX concepts to fulfill the requirements. In terms of a resilient energy system transition, we focused on potential technical, monetary, societal and resource related scale-up limitations.

Within the previous sections it was revealed that the technology of chemical energy storage with PtX processes is generally available. Even consumption of total excess electricity via PtX appears technically feasible. However, costs increase nonlinearly with avoided energy losses, and for all PtX processes high capital expenses have been calculated. This CAPex problem as well as disadvantageous legal framing conditions are considered to currently hinder applications beyond pilot scale and appear to be the most limiting factor for an extensive integration of PtX into energy systems. As an approach for CAPex

Table 5
Comparison of total expenses for the national gas and liquid fuel consumption based on fossil sources and on PtX processes. Calculations are based on mean values from Table 3 and assigned PtX production costs from Fig. 1. Consumption values for 2010 and 2050 are based on an extreme case scenario from the Federal Environment Agency [70].

	Energy source			Energy source	
Final energy consumption 2010	*Natural gas (TWh)*	*Liquid fuel (TWh)*	*Final energy consumption 2050*	*Power-to-Methane (TWh)*	*Power-to-Liquid (TWh)*
	895	696	assumed in *UBA THGND scenario*	587.7	551.9
Fossil	*Natural gas*	*Liquid fuel*	***PtX***	*Natural gas substitute*	*Liquid fuel substitute*
in €kWh^{-1}	0.02	0.06	***in € kWh^{-1}***	0.128 - 0.154	0.154
Total costs (fossil) in billion euros	17.9	41.7	***Total costs (PtX) in billion euros***	75.2 - 90.5	84.9
Sum in billion euros	59.6		***Sum in billion euros***	160.1 - 175.4	

reduction, diminishing storage volumes for hydrogen has been suggested by applying dynamic operation of the processes. On the other hand, this concept drastically enlarges the PtX processes and thereby CAPex of these processes. Furthermore, any dynamic operation requires catalysts with high thermal stability as well as excellent thermo-management to avoid temperature peaks. This includes the usage of platinum group metals, e.g. for PEME, which are considered as scarce resources. Even though reserves might not be considered as critical today, prices could dramatically increase if a worldwide demand for multi GW PtX installations arises. Thus, the availability of scarce raw materials should be further investigated and the catalysts play another key role for cost minimization. This could be possible either by replacing noble metals by more abundant and cheap elements and improving their activity. Especially the latter could allow for process intensification which results in improved space-time yields, i. e. increased throughput and smaller plants.

Another cost factor is process safety: In case of electrolysis it is the mixing risk of getting explosive hydrogen, while the other processes require expensive cooling systems. Decentralized miniplants would therefore require inherent safety concepts. Furthermore, all plants have to be gas-tight which could become a challenge at elevated temperatures. High temperature electrolysis (SOE) profits from external input of heat that might be provided by exothermal processes leading to a high degree of heat integration. In contrary to alkaline electrolysis, PEME provides hydrogen of relatively high purity. The Sabatier reaction, however, requires some purification effort because of limited yield. Depending on the application of methane, residual carbon dioxide might be removed by processes, such as membrane filtration or absorption. The highest effort is required for downstream processing of FTS product streams. In this case cracking and thermal treatment stages are needed. This is not only a fuel quality issue but also determines fuel availability. Finally, fuel availability stands or falls with physical storage capacity, i.e., size of tanks.

Nevertheless, in Chapter 5 it was discussed that high national expenses for PtX processes and the related products always need to be compared with avoided costs of climate change consequences and saved penalty costs for missed climate protection targets, respectively. Given the advantages in the context of contributions to a more resilient energy supply, the additional national energy costs might be considered as economically worthwhile.

In Chapter 3 is was pointed out that further funding for new PtX projects is required to achieve CAPex reduction through scaling effects. According to the requirement of both, flexible operation for grid balancing services as well as large-scale fuel production, we propose more financing of pilot projects as a key mechanism for PtX plant optimization and market integration. The new energy research program of the German government will allow for such new projects [73]. However, business models can hardly develop at current legal framing conditions. Thus, supportive regulations for the production and consumption of renewable electricity based synthetic fuels are also required. Fixed feed-in tariffs might also be discussed as an indirect funding mechanism. Nevertheless, even on a long scale perspective it may be unlikely that PtX products become competitive to today's fossil fuel prices. Higher EU ETS certificate prices or the introduction of carbon taxes for fossil fuels would accelerate economic competitiveness of PtX products.

On a time scale, hydrogen production via electrolysis appears to be the first application of PtX, either for direct use, e.g. hydrogen mobility or integrated in industrial processes for the replacement of SMR. An upscaling progress of electricity based synthetic hydrocarbon production via FTS or Sabatier process is rather important for further proof of concept today, since the share of renewable energy remains too low for a large-scale electricity based synthetic fuel production. However, with increasing renewable energy capacities, all PtX processes are of significant importance and can contribute to sustainably supply all energy sectors with electricity based synthetic fuels, compensate fluctuations of renewable energy supply and increase the resilience of the overall energy system.

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Chapter VII

7. Dynamic Hydrogen Production from PV & Wind Direct Electricity Supply – Modeling and Techno-Economic Assessment

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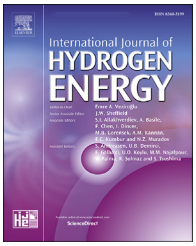

Dynamic hydrogen production from PV & wind direct electricity supply – Modeling and techno-economic assessment☆

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HIGHLIGHTS

- Modeling and simulation of dynamic electrolyzer operation over a period of one year.
- KPI's are reliant on transient power profile and electrolyzer operating flexibility.
- Cheapest hydrogen production costs are 4.33 €/kg for AEL with onshore wind.

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ABSTRACT

Renewable hydrogen from water electrolysis could contribute to the defossilization of various energy intensive sectors but continues to suffer from unfavorable economics. Attention is being paid to the direct supply of renewable electricity to electrolyzers; in particular from photovoltaic (PV) and wind units, whose fixed remuneration period has expired. However, detailed analysis of such operating strategies via modeling and simulation of the dynamic behavior of alkaline electrolysis (AEL) and polymer electrolyte membrane electrolysis (PEMEL) is lacking. In this work, an electrolyzer model is developed for both AEL and PEMEL and analyzed for PV and wind power input data sets from the region of northwest Germany. It is shown that key performance indicators (KPI) such as hydrogen production efficiency, electricity utilization rate, product output and net production costs are highly reliant on the shape of transient power input signals as well as the electrolyzers ability to cope with them. PEMEL technology generally has higher electricity utilization rates than AEL, while AEL still achieves relatively large hydrogen production quantities due to its higher efficiency. Thus, the better operational flexibility of PEMEL cannot generally be considered advantageous in terms of hydrogen production quantities – the same applies for economics. The most competitive hydrogen production costs were 4.33 € per kg for the AEL technology with direct electricity supply from old wind farms, which no longer receive fixed remuneration.

☆ This paper is dedicated to Prof. Dr. Stefan Gößling-Reisemann, who inspired us, shared his knowledge with us and unfortunately cannot be with us today.

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Introduction

Climate change is leading to a transformation of societies towards significant reductions in greenhouse gas emissions (GHG). Especially countries, such as Germany, with a primary energy supply mainly based on fossil sources are facing enormous challenges to reduce GHG emissions in accordance with the Paris Agreement. While the implementation of renewable energies, primarily wind and photovoltaic (PV), already lead to a renewable share of 46.1% in German electricity generation, further expansion requires storage and conversion technologies to compensate for the volatile nature of renewable energy [1,2]. Moreover, the share of renewable energies must increase significantly in other energy intensive sectors like transport, heat and industry as well.

The concepts of power-to-hydrogen and hydrogen-to-x are promising technology paths for both, long-term storage of electricity as well as provision of energy carriers with high energy density to other sectors [3]. In these concepts, water electrolysis is applied to produce hydrogen and is crucial for all power-to-x concepts. Thus, water electrolysis can be considered as a key technology for future energy systems with hydrogen being used directly or as feedstock for the production of hydrocarbon fuels and base chemicals, e.g. ammonia or methanol [4]. The technology of alkaline electrolysis (AEL) is mature and is the current standard for large-scale and steady hydrogen production with capacities of up to 130 MW [5]. New challenges for this technology arise from dynamic operation concepts, e.g. the direct use of volatile power sources or provision of system services for electricity grids as flexible load. Polymer electrolyte membrane electrolysis (PEMEL) is another promising technology regarding flexible operation ability and is being successfully demonstrated in several pilot projects. With a technology readiness level (TRL) of 7–8 it is close to being implemented at an industrial scale, however, the capital costs are still higher than for AEL [6].

For a large-scale implementation, renewable hydrogen needs to become economically viable as compared to other energy carriers or conventional hydrogen from fossil production, e.g. steam methane reforming (SMR) [4]. The electricity costs significantly determine the production costs of hydrogen from electrolysis and are highly dependent on regulative framing conditions. Within the German energy law (EnWG), electrolyzers are legally treated like private households, meaning that several surtaxes are charged over the electricity production costs [7]. Even though several exemptions from paying grid fees and taxes can be achieved, the current EEG reallocation charge of 6.41 ct/kWh$_{el}$ has to be compensated. Alternatively, electrolyzers might operate without a link to the electricity grid, but with a direct connection to a renewable power source. In such a concept the wind or PV farm's electricity production will be primarily utilized by the electrolyzer, whereas unutilized electricity can be fed into the grid (see Fig. 1). This way, the renewable energy law (EEG) reallocation charge may be legally reduced and enable a financially attractive operation strategy with rather low electricity costs [8].

However, there is no long-term experience for such operating concepts, and techno-economic assessment studies are rather generalized without considering in detail the technical limitations of electrolyzers at dynamic operation. In addition, legal framing conditions that apply for direct renewable electricity supply as well as measured power profiles are typically not included in such studies. Decker et al. conduct a techno-economic assessment of hydrogen and e-fuel production from synthesized wind farm profiles for northern Germany. The work is based on integrated modeling of PEMEL, cavern storage, CO_2 capture and fuel synthesis [9]. Matute et al. consider AEL and PEMEL technologies for the provision of grid services for the Spanish electricity grid and evaluate corresponding business cases. Their results show that a flexible electrolyzer operation constitutes to a more profitable hydrogen production [10]. Glenk and Reichelstein investigate hydrogen production from renewables and apply their techno-economic model for case studies in Germany and the USA, taking scaling of the electrolyzers into account [11]. Several further studies, such as [12–16], investigate hybrid energy systems with hydrogen production and assess hydrogen net production costs as well as advantages of renewable electricity utilization via electrolysis.

Overall, detailed techno-economic assessment studies taking into account the technical limitations of electrolyzers at dynamic operation are lacking. Within the framework of this study, an electrolyzer model was developed with the aim of carrying out a profound assessment for hydrogen production with fluctuating electricity feed-in. Detailed modeling allows consideration of ramp speed limitations and specific plant characteristics at partial load operation of both, AEL and PEMEL technology. The model builds on actual electrochemical relationships with a dynamic temperature model as core, on the basis of which further operating variables are

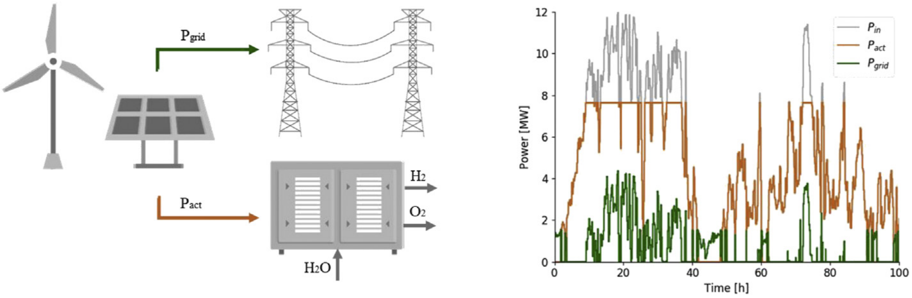

Fig. 1 – Use case electrolysis via direct electricity procurement from wind and PV.

calculated by time-discrete model segments. This approach enables the utilization of different input data sets over a simulation horizon of one year. Besides this long time horizon, the innovation of the proposed approach lies in the merging of electrochemical relationships for cell performance and the temperature model from Ulleberg [17] with the plant periphery. The considered electrochemistry is primarily based on Abdin et al., Hammoudi et al. and Henao et al. for AEL modeling [18–20] and Chandesris et al., Tjarks and Abdin et al. for PEMEL modeling [21–23]. Only a limited number of integrated modeling approaches for AEL and PEMEL have been published so far. The two prior mentioned papers by Abdin et al., one of which is dedicated to PEMEL and one to AEL, as well as the work of Fragiacomo et al. are an exception [18,23,24].

A script-based analysis of hydrogen production economics is carried out on basis of the determined operating characteristics. The simulations are applied for onshore and offshore wind farms and a west-east orientated PV plant, all located in the region of northwest Germany. The techno-economic assessment covers considerations of specific electricity procurement costs for the individual power sources.

Methodology

A model for both, AEL and PEMEL, has been developed and implemented in Python with the aim to simulate realistic electrolyzer characteristics in transient operation. This work considers four different power input data sets, representing different direct renewable electricity supply scenarios. In the following subsections the setup of the electrolyzer model is discussed (Section Electrochemical fundamentals and modeling of AEL and PEMEL), followed by a characterization of the individual electricity input signals (Section Power input data sets) and an introduction to the electrolyzer scaling considered (Section Electrolyzer scaling). The approach for the techno-economic assessment is introduced in Section Techno-economic analysis, including a listing of the relevant assumptions.

Electrochemical fundamentals and modeling of AEL and PEMEL

The dissociation of water in an electrolyzer is represented by a spatially separated redox reaction with an oxidization reaction at the anode side (oxygen evolution reaction, OER) and a reduction reaction at the cathode side (hydrogen evolution reaction, HER). However, AEL and PEMEL differ in types of charge carriers and electrolytes. Whereas OH^- ions move from the anode side to the cathode in AEL, H^+ ions move from cathode to anode in PEMEL (Table 1). A certain electrode- or cell potential is required for electrode reactions to occur, which is achieved by applying an external voltage to the electrochemical cell. When neglecting parasitic currents, the amount of product gas obtained is directly proportional to the present cell current. The lower the cell voltage required to achieve a specific cell current, the higher the cell efficiency or the lower the specific energy demand. To determine the energy demand of a cell or its specific energy requirement, voltage and current must be determined at a dedicated operating point. Plotting u_{cell} against i_{cell} yields the characteristic polarization curve of an electrochemical cell.

Electrolysis plants are typically built of several stacks with a specific number of cells and technology specific electrochemical properties. The stacks are supplemented by auxiliary components such as feed-water purification, pre-heaters, power-electronics (rectifier and operation control), gas purifier and dryer and product gas compression. The developed model is based on individual cell- and auxiliary characteristics adopted from recent literature. Parameterization does not reflect a specific electrolyzer but rather a representative example of an electrolyzer type. The core of the simulation program is built of two nested loops. The outer loop imports the net power input for each time interval and generates output data sets, while the inner loop calculates the actual electrochemical cell characteristics (compare Fig. 2).

The optimum operating point of the electrolyzer is primarily dependent on cell temperature and available power input. It is determined from the polarization curve for each time increment using an optimization solver. As illustrated in Fig. 2, the available power input to the stack P_{diff} is calculated by the difference of signal input P_{in} and peripheral power consumption P_{aux}, whereby P_{aux} takes into account the gas drying P_{tsa}, the pumping of cooling and reactant water P_{pmp} and electrolyte pumping P_{ely} (P_{ely} is only relevant for AEL). The peripheral power consumption is considered to be inert, so that output values of the preceding time step can be used. The dynamic behavior of the electrolyzer is approximated by means of maximum permitted power gradients, being represented by the P_{grad} function. The P_{grad} function as well as the efficiency of the power electronics are considered in order to determine the actual power consumption of the stack P_{st} on basis of P_{diff}. The power consumption on system level P_{act} is made up of the sum of P_{aux} and P_{st}. Within the described calculation sequence, the efficiency of the power electronics and other peripheral components are considered in dependency of the operating point.

Table 2 displays relevant technical input parameters for AEL and PEMEL. The PEMEL technology approves a more flexible operating characteristic in terms of load-flexibility and ramp-speed. The most relevant electrochemical and technical correlations for the model setup are described below.

Table 1 – Basic technology information for AEL and PEMEL.

Technology	Cathode reaction	Anode reaction	Charge carrier	Electrolyte
AEL	$H_2O + 2e^- \rightarrow H_2 + 2OH^-$	$2OH^- \rightarrow 0.5O_2 + H_2O + 2e^-$	OH^-	Aqueous KOH solution
PEMEL	$2H^+ + 2e^- \rightarrow H_2$	$H_2O \rightarrow 0.5O_2 + 2H^+ + 2e^-$	H^+	Solid polymer

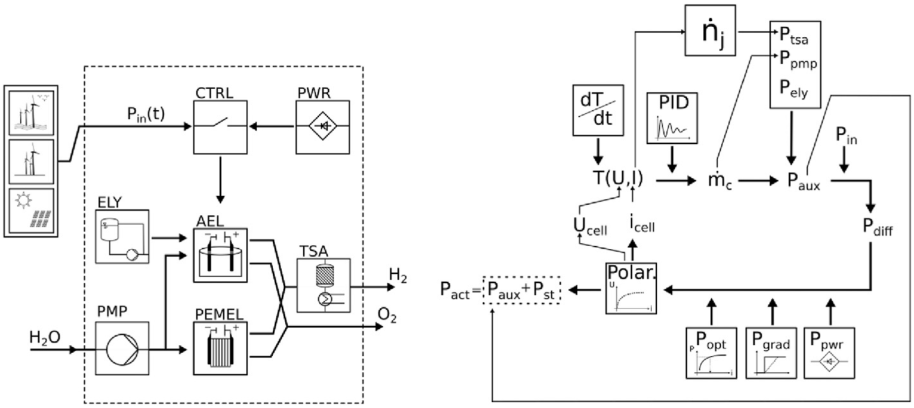

Fig. 2 – Model structure (left: components considered by the model; right: detailed representation of the inner loop implementation).

Table 2 – Technical model input parameters for AEL and PEMEL electrolysis [6,25,26].

	AEL	PEMEL	Unit
Target stack temperature	80	80	°C
Load flexibility	20–100	5–100	$\%P_N$
Ramp-speed	1.67	10	$\%P_N/s$

Product output

Molar product gas yield of species i ($\dot{n}_i$) is, on the basis of Faraday's law, directly proportional to a cell's current density i_{cell}:

$$\dot{n}_i = \frac{i_{cell} \cdot A_{cell}}{z \cdot F} \tag{1}$$

Cell voltage

The thermodynamically minimum energy to be applied for water splitting is expressed by the free Gibbs enthalpy or the so-called reversible cell voltage [3]:

$$-\Delta E_0 = \frac{\Delta G}{z \cdot F} = \frac{\Delta H - T \cdot \Delta S}{z \cdot F} \tag{2}$$

Deviations from standard conditions and consideration of the activity of reactants and products are provided by the so-called Nernst-voltage, yielding the open-circuit potential. The ratio of the activities is represented by the ratio of the corresponding partial pressures:

$$U_{oc} = -\Delta E = \frac{\Delta G}{z \cdot F} + \frac{RT}{zF} \ln \frac{p_{O_2}^{0.5} p_{H_2}}{p_{H_2O}} \tag{3}$$

Partial pressure

The partial pressure calculation is carried out in accordance with [22,27] and application of index j, which represents the anodic or cathodic cell compartment:

$$p_i^j = p^j - p_{H_2O,s} \tag{4}$$

The product gases are assumed to be saturated with water vapor. For AEL the water vapor pressure is calculated according to Ref. [18,28], considering the molality of the potassium hydroxide electrolyte b_{KOH}:

$$\begin{aligned} \log\left(p_{H_2O,KOH}\right) = & -0.01508 \cdot b_{KOH} - 0.0016788 \cdot b_{KOH}^2 \\ & + 2.25887 \cdot 10^{-5} \cdot b_{KOH}^3 + \big(1 - 0.0012062 \cdot b_{KOH} \\ & + 5.6024 \cdot 10^{-4} \cdot b_{KOH}^2 - 7.8228 \cdot 10^{-6} \cdot b_{KOH}^3\big) \\ & \cdot (35.4462 - 3343.93/T - 10.9 \cdot \log(T) + 0.0041645 \cdot T) \end{aligned} \tag{5}$$

For the PEMEL, the partial pressure calculation is supplemented by a summand of a current density dependent partial pressure increase, with A_{p-enh}^j being an experimentally determined factor [29], while the water vapor pressure is calculated temperature dependent [27]:

$$p_i^j = p^j - p_{H_2O,s} + i_{cell} \cdot A_{p-enh}^j \tag{6}$$

$$p_{H_2O,s} = 6.1078 \cdot 10^{-3} \cdot \exp\left(17.2694 \cdot \frac{T - 273.15}{T - 34.85}\right) \tag{7}$$

Overpotential

In addition to the reversible cell potential, the initialization of the electrochemical reaction requires a so-called "overpotential", being dependent on the properties of the electrodes, the catalyst and the material flow. The activation overpotential results from the reaction kinetics of the electrodes (theory of the activated complex). The relation between activation overpotential and current density is expressed by the Butler-Volmer equation:

$$i = i_0 \cdot \left(\exp\left(\frac{-\alpha \cdot z \cdot F}{R \cdot T} \cdot \eta\right) - \exp\left(\frac{(1-\alpha) \cdot z \cdot F}{R \cdot T} \cdot \eta\right)\right) \tag{8}$$

The electrode or catalyst activity is represented by the exchange current density i_0, which is calculated differently for AEL and PEMEL. For AEL, the following equations are applied for calculation of the exchange current density and the activation overpotential [18]:

$$i_0^j = \gamma^j \cdot \exp\left[-\frac{E_{akt.}^j}{R} \cdot \left(\frac{1}{T} - \frac{1}{T_{ref}^j}\right)\right] \cdot i_{0,ref}^j \tag{9}$$

$$\eta^{j}_{act} = \frac{RT}{\alpha^{j}F} \cdot \ln\left(\frac{i_{cell}}{i^{j}_{0}(1 - \Theta^{j})}\right) \tag{10}$$

Herein Θ^{j} represents a bubble cover factor (reduction of active surface). The exchange current density and the activation overpotential for the PEMEL are calculated as follows [21]:

$$i^{j}_{0} = z \cdot F \cdot k^{j}_{0} \cdot T \cdot \exp\left(-\frac{E^{j}_{act.}}{RT}\right) \tag{11}$$

$$\eta^{An}_{act} = (R \cdot T) / (\alpha^{An} \cdot z \cdot F) \cdot \log\left(\frac{i_{cell}}{i^{An}_{0} \cdot \gamma^{An}}\right) \tag{12}$$

In this work, the concentration overpotential is neglected. This is in line with other literature and admissible, since its contribution is small, especially with low current densities [30]. However, further inhibition is considered in terms of ohmic resistances of separator, membrane and electrolyte. For AEL, this phenomenon is taken into account using the following mathematical relationships [18,20]:

$$\eta^{j}_{\Omega,el} = i_{cell} \cdot A_{cell} \cdot \frac{1}{\sigma_{ni}} \cdot \frac{\delta^{j}_{el}}{A^{j}_{el}} \tag{13}$$

$$\eta_{\Omega,ely,\Theta} = i_{cell} \cdot A_{cell} \cdot \frac{1}{\sigma_{KOH,free}} \cdot \left(\frac{l^{An}_{sep-el}}{A^{An}_{el}} + \frac{l^{Ka}_{sep-el}}{A^{Ka}_{el}}\right) \cdot \left(\frac{1}{\left(1 - \frac{2}{3}\Theta\right)^{3/2}} - 1\right) \tag{14}$$

$$\eta_{\Omega,sep} = i_{cell} \cdot A_{cell} \cdot \frac{\rho_{sep}\tau^{2}_{sep}\delta_{sep}}{\omega_{sep}\varepsilon_{sep}A_{sep}} \tag{15}$$

For the PEMEL, the transition resistances at the current collectors are taken into account besides the temperature-dependent membrane resistance [21]:

$$\eta_{\Omega} = i_{cell} \cdot A_{cell} \cdot R_{\Omega} \tag{16}$$

$$R_{\Omega} = \frac{\delta_{mem}}{\sigma_{mem}} + \frac{\delta^{an}_{ccoll}}{\sigma^{an}_{ccoll}} + \frac{\delta^{ca}_{ccoll}}{\sigma^{ca}_{ccoll}} \tag{17}$$

$$\sigma_{mem} = 0.005139\lambda - 0.00326\left[1268 \cdot \left(\frac{1}{303} - \frac{1}{T}\right)\right] \tag{18}$$

Material balance

Similar to other modeling approaches, the model is based on a simplified material balance, neglecting permeation and other material losses [18,21,23,24]. Permeation processes within electrolysis cells, e.g. diffusion, water drag et cetera, may lead to specific gas contamination, which results in a more complex material balance. A widespread assumption for the cathode side is that permeated oxygen immediately reacts with hydrogen [22]. Thus, product gas contamination can be considered negligible. However, higher hydrogen concentrations at the anode side may exceed the lower explosion limit of H_2/O_2 gas mixture. For safety reasons electrolyzers are typically shut down at a "H_2 in O_2" concentration of ≥2 vol.-%. Within the PEMEL model the evaluation of the "H_2 in O_2" concentration is simplified according to Ref. [22].

Temperature model

For both electrolysis technologies the thermo-model of Ulleberg is implemented (eq. (19–23)), with the assumption of a lumped heat capacity C_t and a homogeneous heat distribution within each stack [17]. The core of Ulleberg's thermo-model is a linear ordinary differential equation (eq. (19)), which is composed of the terms α and β with the time constant τ_t and the heat capacity of the coolant C_c. In accordance with Ulleberg and Gabrielli et al., heat generation through overpotentials, heat losses to the ambiance and heat losses to the cooling water stream are considered [17,31].

$$\frac{dT}{dt} = -\alpha T + \beta \tag{19}$$

$$\alpha = \frac{1}{\tau_t} + \frac{C_c}{C_t}\left[1 - \exp\left(\frac{-A_{hx}H_{hx}}{C_c}\right)\right] \tag{20}$$

$$\beta = \frac{NI_{cell}(U_{cell} - U_{tn})}{C_t} + \frac{T_a}{\tau_t} + \frac{C_c T^{i}_{c}}{C_t}\left[1 - \exp\left(\frac{-A_{hx}H_{hx}}{C_c}\right)\right] \tag{21}$$

$$\tau_t = R_t C_t \tag{22}$$

$$C_c = \dot{m}_c c_{p_c} \tag{23}$$

The stack temperature is controlled via a PID controller, which is related to the cooling water mass stream of AEL and PEMEL, respectively.

Performance and efficiency factor

An electrolysis cell's characteristic is typically related to cell current density i_{cell} and cell potential U_{cell} and can be plotted in a polarization curve. Fig. 3 shows the polarization curves of AEL and PEMEL. For PEMEL, the curve follows the experimental data of Chandesris et al. [21] adequately, while the AEL polarization curve compares well to the work of Abdin et al. [18]. However, the comparison with the reference shows that the AEL model represents a slightly conservative performance in the lower partial load range. This is of minor relevance for the analysis, since the AEL does not operate below 20% P_N.

Since the electrical power consumption of a cell corresponds to the product of current and voltage, the cell power increases with increasing overvoltages and ohmic losses at constant gas production. Consequently, due to the characteristic polarization curves of electrolyzers, the cell efficiency increases with decreasing current density or decreasing cell power. An efficiency maximum is reached in the lower part-load range, which has also been demonstrated by electrolyzer operation [32].

Power input data sets

Four input signals for renewable energy generation, being characterized in Table 3, are utilized for simulation of the electrolyzers' long-term operating behavior: A signal, which represents a PV farm running out of its fixed remuneration period, an "old" onshore wind farm running out of its fixed

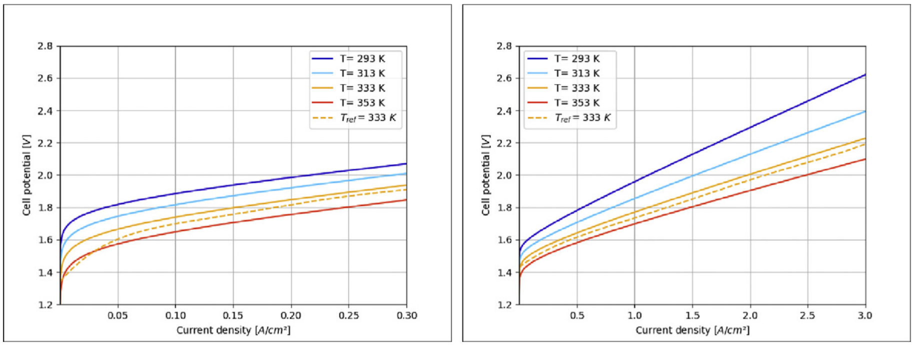

Fig. 3 – Simulated polarization curve of the AEL (left) and PEMEL (right) with reference data from Abdin et al. and Chandesris et al., respectively [18,21].

Table 3 – Input signal properties.

	PV farm	Onshore wind farm "up-to-date"	Onshore wind farm "old"	Offshore wind farm
Plant type [–]	SolarFrontier SF 150-S	Vestas V90	AN Bonus N70	Siemens SWT-3.6
Data resolution [min]	15	10	10	10
Peak power per unit [MW]	0.00015	2	2	3.6
Total peak power [MW]	0.25	12.01	12.16	400.00
Electricity generated [MWh/a]	237.27	28,234.13	16,095.93	1,235,124.17
Full load hours [h]	961	2352	1324	3088

remuneration period, an "up-to-date" onshore wind farm and an offshore wind farm. All the renewable energy generation profiles considered were measured in northwest Germany in 2017. The data sets for PV, onshore wind farm "up-to-date" and offshore wind farm have been scaled linearly for reasons of confidentiality.

Fig. 4 shows the power generation profiles of the different data sets. Differences in the peak power as well as in the shape of PV and wind turbine profiles can be observed. The PV data set shows an expected seasonal fluctuation of the peak power depending on ecliptic and radiation. No clear seasonal trends are discernible within the wind turbine profiles. However, all wind farm performance curves reflect consistent wind conditions. The respective annual load duration curves, shown in Fig. 5, indicate that the proportion of certain partial load ranges differs considerably from signal to signal. The "up-to-

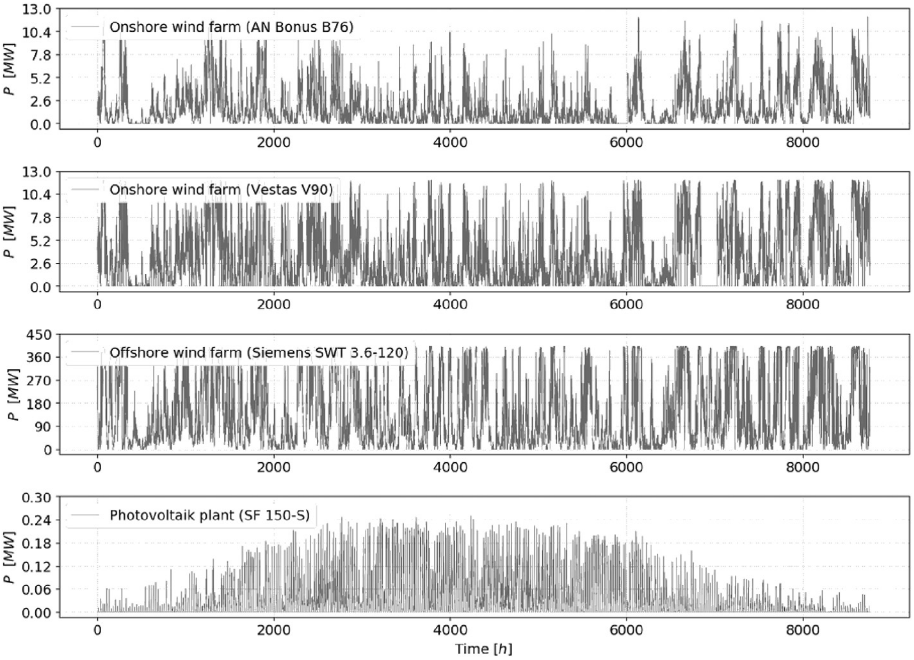

Fig. 4 – Analyzed power generation profiles.

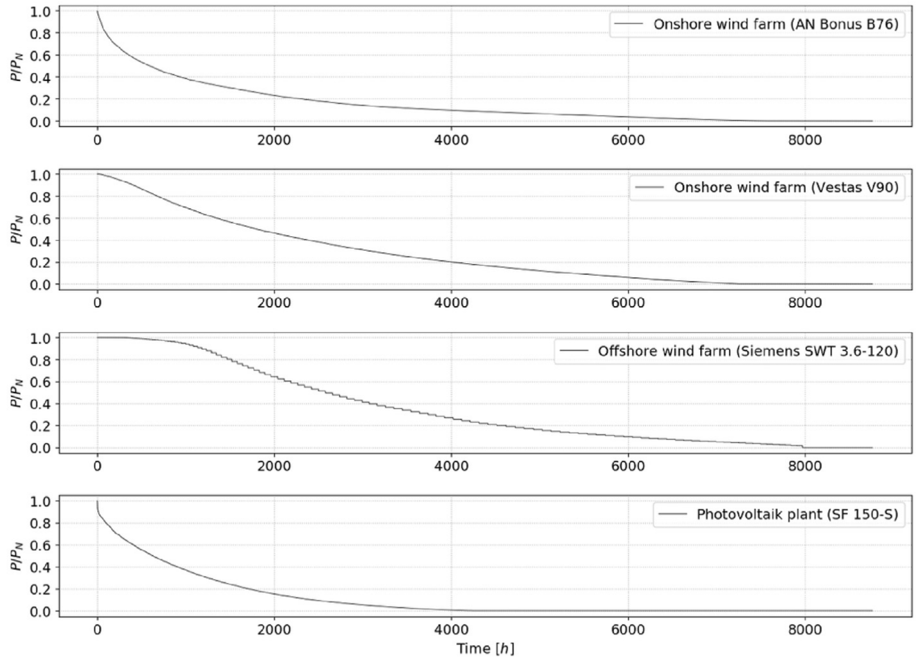

Fig. 5 – Annual load duration curves of the four power input profiles.

date” wind farm and especially the offshore wind farm have a significantly higher share in the full-load or high-load range and thus a better yield than the “old” onshore wind farm and the PV farm.

Electrolyzer scaling

Simulations are carried out for different nominal loads (P_N) of the electrolyzer. The stack capacities are scaled to 40%, 60% and 80% of the maximum power input ($P_{in,max}$). The resulting total electrolyzer system capacity is slightly higher due to additional power consumption of peripheral components. For each technology, an upper stack capacity is defined, being 2 MW for PEMEL and 4 MW for AEL [25]. With a minimum number of stacks, the number of cells per stack is constant for the different scaling variants. The cell areas are taken from published parameter sets [18,31]. By using uniform stack sizes for each case (constant number of cells per stacks for each scaling and technology), slight deviations in system power between AEL and PEMEL occur. The resulting electrolyzer scaling is displayed in Table 4.

Techno-economic analysis

The techno-economic analysis is based on a standard methodology by Peters et al. [33], with all costs classified either as capital expenditures (CAPEX) or as operational expenditures (OPEX). The calculation of the total CAPEX builds on the electrolyzers bare acquisition costs, which are divided into acquisition costs for the stack (C_{Stack}) and the balance of plant (C_{BoP}). A ratio factor (RF) of 1.54 is applied to account for further capital investment, including installation, yard improvements, legal expenses, contractor fees and contingencies [9,34]. The RF is lower in comparison to thermochemical processes, since electrolyzers are delivered as skid-mounted units.

$$\text{CAPEX}\ [€] = \text{CAPEX}_{BoP} + \text{CAPEX}_{Stack} = \text{RF} \cdot (C_{BoP} + C_{Stack}) \qquad (24)$$

The maturity of AEL technology leads to rather low CAPEX of 770 €/kW for an AEL electrolysis system compared to PEMEL technology with 1324 €/kW. However, maintenance expenses are higher for AEL electrolyzers, which is inter alia due to the liquid electrolyte cycle. The corresponding economic input parameters are shown in Table 5.

Table 4 – Electrolyzer plant parameters.

		40% $P_{in,max}$		60% $P_{in,max}$		80% $P_{in,max}$	
		AEL	PEMEL	AEL	PEMEL	AEL	PEMEL
PV farm	Stacks [–]	1	1	1	1	1	1
	Power [kW]	100.5	100.5	149.7	149.7	200.1	200.0
Onshore wind farms	Stacks [–]	2	3	2	4	3	5
	Power [MW]	4.8	4.8	7.2	7.2	9.6	9.6
Offshore wind farm	Stacks [–]	40	82	60	122	80	163
	Power [MW]	160.1	160.1	240.1	240.1	320.1	320.1

Table 5 – Economic model input parameters for AEL and PEMEL electrolysis.

	Symbol	Unit	AEL	PEMEL	Literature
Acquisition costs	C	€/kW	500	860	[34,35]
Stack's share of acquisition costs	–	%	45.4	48.0	[6]
Service and maintenance costs	K_{SaM}	€/(a·kW)	19	13	[6]
Stack overhaul period	OP	$h_{Operation}$	60,000	44,200	[6,35]
System lifetime	SL	a	20		
Interest rate	IR	%	5		
Deionized water	K_{H2O}	€/m^3	1		[36]
Taxes and insurances	K_{TaI}	a^{-1}	0.02		[33]

Table 6 – Economic comparison of different electricity input signals. For each signal, the electricity procurement costs are stated with and without partial EEG surcharge [37–39].

	Electricity procurement costs excl. surcharge [ct/kWh]	Electricity procurement costs incl. surcharge [ct/kWh]
PV	4.5	5.8
Onshore wind farm "up-to-date"	9.3	10.6
Onshore wind farm "old"	4.5	5.8
Offshore wind farm	15.4	16.7

The annualized capital expenditures (ACAPEX) are calculated according to Eq. (25) as a function of CAPEX, interest rate (IR) and system lifetime (SL).

$$ACAPEX\left[\frac{€}{a}\right]=CAPEX\cdot\frac{(IR+1)^{SL}\cdot IR}{(IR+1)^{SL}-1} \tag{25}$$

The OPEX consider service and maintenance, stack replacements, insurances, taxes, electricity supply and supply with deionized water. Remote monitoring of the automated process is assumed and therefore regular labor costs are neglected. Stack replacements or major stack overhauls are required after a certain stack overhaul period (OP). Accordingly, the total number of stack replacements required per system lifetime depends on the annual operating hours (OH) and thus on the operation mode. Eq. (26), which considers natural numbers of replacements per system lifetime, is applied for calculation of the replacement costs (K_R). This procedure ensures that dynamic operation is also considered in the TEA and reflects that higher operating hours require an earlier stack replacement.

$$K_R\left[\frac{€}{a\cdot kW}\right]=\frac{C_{Stack}}{SL}\cdot\left[\frac{SL\cdot OH}{OP}-1\right] \tag{26}$$

$$OPEX\left[\frac{€}{a}\right]=\dot{V}_{H_2O}\cdot K_{H_2O}+W_{el}\cdot K_{el}+P_N\cdot K_{SaM}+CAPEX\cdot K_{TaI}+P_N\cdot K_R \tag{27}$$

As result of the TEA, the net production costs (NPC) of hydrogen are calculated by division of the annualized production expenditures by the annual product output (PO).

$$NPC\left[\frac{€}{Nm^3}\right]=\frac{ACAPEX+OPEX}{PO} \tag{28}$$

The applied electricity procurement costs (K_{el}) are shown in Table 6. For both, the PV and onshore wind farm "old" signal, levelized costs of electricity of 4.5 ct/kWh$_{el}$ are considered, whereas the onshore wind farm "up-to-date" as well as the offshore wind farm receive a revenue of 9.3 ct/

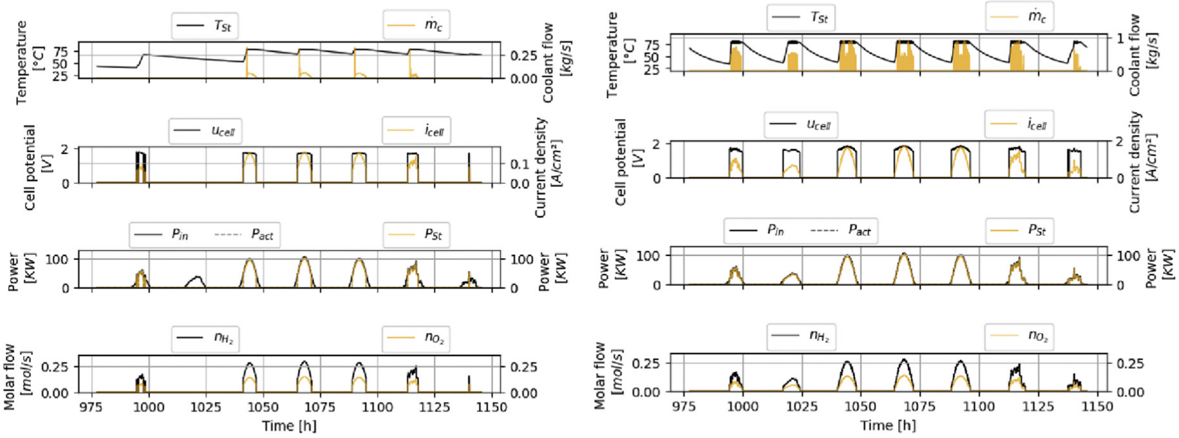

Fig. 6 – Simulated characteristics of AEL (left) and PEMEL (right) technologies in 80% scale of $P_{in,max}$ and in relation to the PV power input signal for an average summer week.

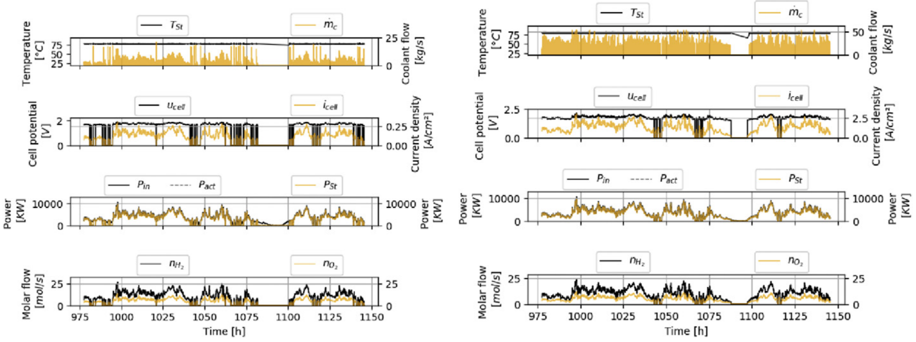

Fig. 7 – Simulated characteristics of AEL (left) and PEMEL (right) technologies in 80% scale of $P_{in,max}$ and in relation to the "up-to date" wind farm power input signal for an average summer week.

kWh$_{el}$ and 15.4 ct/kWh$_{el}$ via a fixed subsidization tariff (EEG remuneration) [37,38]. Furthermore, the input electricity for power-to-x processes is regularly surcharged by the EEG reallocation charge of currently 6.41 ct/kWh$_{el}$. However, electrolyzers may legally operate with a reduced EEG reallocation charge of 1.3 ct/kWh$_{el}$ [8]. All simulations compare electrolysis operation with the basic electricity procurement costs as well as a combination of basic electricity procurement costs plus reduced EEG reallocation charge.

Results and discussion

The simulation results are split into two sections. In Section Operating characteristics, the simulated operating characteristics are presented and discussed, while Section Techno-economics focuses on the results of the techno-economic evaluation, which are based on the mass and energy balances obtained by simulation.

Operating characteristics

Fig. 6 and Fig. 7 display operational characteristics of the simulated AEL and PEMEL technologies in 80% scale for the PV and "up-to-date" wind power signals over a time interval of one week. Functionality of the thermo-model and control is approved by the trend of stack temperature T_{ST} and cooling waterflow $\dot{m}_c$ according to the power input P_{in}. The comparison of power input, actual power of the electrolyzer P_{act} and stack power P_{st} shows valid results, as the maximum electrolyzer power does not exceed 80% of $P_{in,max}$. The material balances of product gases show an expected molar ratio of 2:1 (H_2/O_2) with a proportional trend to P_{st} and current density.

The number of operation hours of AEL and PEMEL electrolyzers are strongly dependent on the flexibility potential of the technologies. For the PV input signal, the AEL achieves 1868 operation hours, PEMEL operates 3111 h/a instead. However, the significantly longer operation time of PEMEL results in low benefits in terms of hydrogen production with 4.39 t/a at 1148 annual equivalent full load hours (FLH) for PEMEL and 4.02 t/a at 1004 FLH for AEL, respectively. This can be explained by a comparably frequent operation at the lower part load range of the PEMEL in times of low electricity generation, whereas the AEL does not operate at these conditions due to its lower part load limit of 20% of P_N. Furthermore, the PEMEL technology benefits from its higher ramping speed (see Table 2). 97.3% of the PV input electricity can be utilized by PEMEL and 84.7% by AEL.

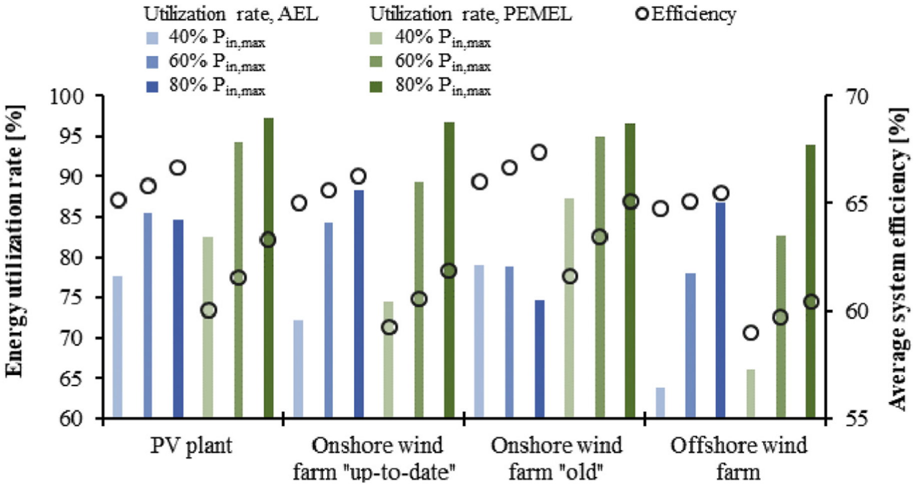

Fig. 8 – Electricity utilization rate and electrolyzer system efficiency based on LHV_{H2}.

Table 7 – Comparison of hydrogen production values in relation to electricity generation signal.

Input signal	Electrolyzer scaling	AEL Utilized electricity	AEL FLH	AEL Hydrogen production	PEMEL Utilized electricity	PEMEL FLH	PEMEL Hydrogen production
[–]	[% of $P_{in,max}$]	[MWh]	[h/a]	[t/a]	[MWh]	[h/a]	[t/a]
PV	40	184.1	1832.6	3.6	195.7	1946.6	3.5
PV	60	203.0	1355.8	4.0	223.6	1492.9	4.1
PV	80	200.9	1003.8	4.0	230.8	1148.0	4.4
Onshore “up-to-date”	40	20372.9	4244.2	397.4	21052.1	4385.5	374.5
Onshore “up-to-date”	60	23775.7	3301.9	468.1	25235.5	3504.6	458.7
Onshore “up-to-date”	80	24952.5	2597.8	496.1	27316.7	2844.0	507.4
Onshore “old”	40	12729.5	2651.9	252.1	14056.2	2928.1	259.9
Onshore “old”	60	12681.1	1761.1	253.6	15289.4	2123.3	291.1
Onshore “old”	80	12029.7	1252.4	243.3	15528.8	1616.7	303.3
Offshore	40	787792.1	4921.7	15319.6	816862.4	5103.2	14456.8
Offshore	60	963146.4	4011.3	18820.6	1022493.2	4258.5	18328.6
Offshore	80	1071320.9	3346.9	21047.5	1159965.6	3623.8	21044.6

Total operation time differs even more at the “up-to-date” onshore wind signal where PEMEL operates 6261 h and AEL 4333 h. In this case, 3282 MWh_{el} cannot be utilized by AEL compared to 917 MWh_{el} by PEMEL. However, this does not result in a significantly higher hydrogen production with 507.4 t/a compared to 496.1 t/a by AEL. Whether the higher flexibility and better electricity utilization rate of PEMEL can be considered economically beneficial is dependent on techno-economic parameters and subject of Section Techno-economics.

Fig. 8 shows the share of the generated electricity that is utilized by the electrolyzer as well as its average efficiency for all input signals and scalings. A clear trend towards higher efficiencies can be observed with increased scaling (40% $P_{in,max}$ to 60% $P_{in,max}$ to 80% $P_{in,max}$) for both AEL and PEMEL and all input signals. This is due to various superimposed effects, two of which are described in the following. The first is that cell efficiency and thus system efficiency increases with a decreasing ratio of effective load to nominal load, which is due to lower current densities. With the same signal, the share of operation in the lower part-load range tends to increase with the electrolyzer capacity. Apart from that, an increasing (nominal) load results in a decrease of the relative energy demand of the peripheries. It can be derived that the shape of the input signal in conjunction with the electrolyzer scaling directly influences the efficiency of hydrogen production, while the specific energy consumption is generally lower for AEL.

Besides, Fig. 8 illustrates that the share of the electricity utilized with a certain signal and scaling is generally higher for PEMEL than for AEL. However, the utilization rate does not show a clear trend depending on the scaling. While an increase in energy utilization rate with scaling is determined for the considered cases with PEMEL technology, the opposite picture emerges for AEL technology with the onshore wind farm “old” signal, having its maximum at a scaling of 40% of $P_{in,max}$. For AEL with the PV signal, maximum energy is utilized with an electrolyzer scaling of 60% of $P_{in,max}$. Therefore, it cannot be generalized that an electrolyzer with higher nominal load allows the conversion of more electricity into

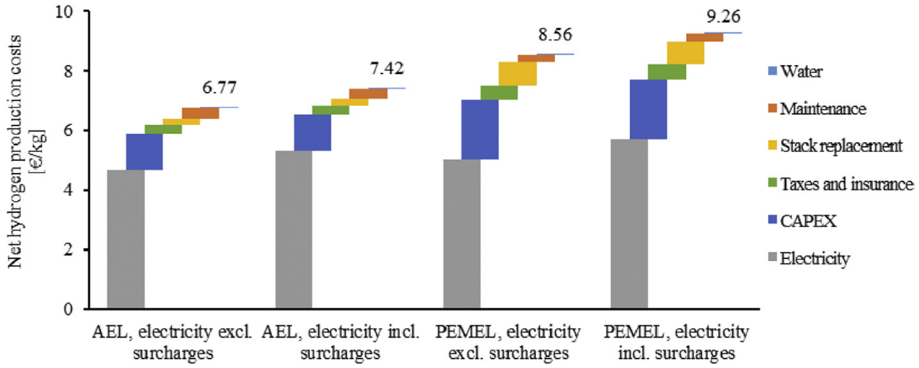

Fig. 9 – Breakdown of the net hydrogen production costs for AEL and PEMEL in 80% scale of $P_{in,max}$ and in relation to the “up-to date” onshore wind farm power input signal.

Table 8 – Breakdown of hydrogen net production costs for AEL technology.

Input signal and electrolyzer scaling	CAPEX [€/kg]	Maintenance [€/kg]	Electricity excl. surcharge [€/kg]	Electricity incl. surcharge [€/kg]	Stack overhaul [€/kg]	Taxes and Insurance [€/kg]	Water [€/kg]	H_2 NPC excl. surcharges [€/kg]	H_2 NPC incl. surcharges [€/kg]
PV 40% $P_{in,max}$	1.72	0.53	2.30	2.97	0.00	0.43	0.01	5.00	5.66
PV 60% $P_{in,max}$	2.31	0.71	2.28	2.94	0.00	0.58	0.01	5.88	6.54
PV 80% $P_{in,max}$	3.08	0.95	2.25	2.90	0.00	0.77	0.01	7.05	7.70
Onshore “up-to-date” 40% $P_{in,max}$	0.75	0.23	4.77	5.43	0.14	0.19	0.01	6.08	6.74
Onshore “up-to-date” 60% $P_{in,max}$	0.95	0.29	4.72	5.38	0.17	0.24	0.01	6.39	7.05
Onshore “up-to-date” 80% $P_{in,max}$	1.20	0.37	4.68	5.33	0.22	0.30	0.01	6.77	7.42
Onshore “old” 40% $P_{in,max}$	1.18	0.36	2.27	2.93	0.22	0.29	0.01	4.33	4.99
Onshore “old” 60% $P_{in,max}$	1.75	0.54	2.25	2.90	0.32	0.44	0.01	5.31	5.96
Onshore “old” 80% $P_{in,max}$	2.44	0.75	2.22	2.87	0.00	0.61	0.01	6.03	6.67
Offshore 40% $P_{in,max}$	0.65	0.20	7.92	8.59	0.24	0.16	0.01	9.17	9.84
Offshore 60% $P_{in,max}$	0.79	0.24	7.88	8.55	0.14	0.20	0.01	9.26	9.93
Offshore 80% $P_{in,max}$	0.94	0.29	7.84	8.50	0.17	0.23	0.01	9.48	10.14

hydrogen. This is primarily since with a larger nominal load, the lower load range in which the electrolyzer cannot be operated also increases in absolute terms. With a larger scaling of the electrolyzer, higher peaks in generation can be utilized, while on the other hand downtimes increase. Consequently, it depends on the flexibility properties of the electrolyzer as well as the shape of the input signal whether a higher electrolyzer capacity allows the production of more hydrogen. This phenomenon is particularly relevant for alkaline electrolyzers with direct electricity supply from PV or “old” onshore wind farms, as the corresponding electricity generation profiles have a relatively high share in their low part-load range, in which operation of AEL is more restricted than PEMEL.

Table 7 provides the utilized electricity, achieved electrolyzer FLH and the corresponding quantity of hydrogen produced. An interesting finding is that AEL achieves relatively large hydrogen production quantities despite its lower electricity utilization rate compared to PEMEL. This is especially applicable for the input signals of modern renewable energy plants. It can be attributed to the higher efficiencies of AEL in accord with the more favorable electricity production patterns of the “up-to-date” onshore wind farm and the offshore wind farm with less operating hours in the lower part-load range. Thus, the better flexibility of PEMEL cannot generally be considered advantageous in terms of hydrogen production quantities.

Techno-economics

The techno-economic assessment is carried out based on the parameters presented in Section Techno-economic analysis. A comparison of the breakdown of the net hydrogen production costs for AEL and PEMEL technology is shown in Fig. 9. For this purpose, the results for the “up-to-date” wind farm power input signal with 80% scale of $P_{in,max}$ are selected. For both technologies, the electricity purchase has by far the highest share with 69.1% for AEL and 58.5% for PEMEL, while considering electricity procurement without surcharges (71.8% and 61.6% incl. surcharges). This is followed by the capital expenditures with shares of 17.7% and 23.5% (16.1% and 21.7% incl. surcharges). The absolute contributions of these parameters are higher for PEMEL, which is due to higher specific investment costs per MW as well as a lower efficiency and is in accord with standard literature. While the relatively low shares for water, taxes and insurances as well as maintenance costs for both technologies are of the same order of magnitude, the result is particularly interesting with regard to the stack replacement costs. Due to a shorter stack overhaul period and higher operation hours, two major overhauls must be carried out for the PEMEL instead of one for the AEL. In conjunction with higher costs per replacement, this leads to significant higher stack replacement costs, which account for 3.2% of the NPC for AEL and 9.1% for PEMEL, respectively (3.0% and 8.4% incl. surcharges). The cost breakdown for all cases considered are provided in Table 8 for AEL and Table 9 for PEMEL.

Hydrogen net production costs for electricity procurement without surcharges are illustrated in Fig. 10 for all input signals and AEL as well as PEMEL technology. It can be observed that AEL achieves lower production costs for each input signal and scaling compared to PEMEL. Apart from that, it can be generalized for both technologies and all input signals that a smaller electrolyzer scale leads to higher operation hours as well as lower hydrogen production costs. In contrast to the PV or the “old” onshore wind farm signal, a relatively high electrolysis capacity can tend to be selected for current wind farms, without having to accept significant losses for the NPC.

Fig. 10 shows that from an economic point of view, a direct electricity purchase from renewable electricity units running

Table 9 – Breakdown of hydrogen net production costs for PEMEL technology.

Input signal and electrolyzer scaling	CAPEX	Maintenance	Electricity excl. surcharge	Electricity incl. surcharge	Stack overhaul	Taxes and Insurance	Water	H_2 NPC excl. surcharges	H_2 NPC incl. surcharges
	[€/kg]	[€/kg]	[€/kg]	[€/kg]	[€/kg]	[€/kg]	[€/kg]	[€/kg]	[€/kg]
PV 40% $P_{in,max}$	3.03	0.37	2.50	3.22	0.59	0.75	0.01	7.25	7.98
PV 60% $P_{in,max}$	3.85	0.47	2.44	3.14	0.75	0.96	0.01	8.48	9.19
PV 80% $P_{in,max}$	4.87	0.60	2.37	3.05	0.95	1.21	0.01	10.01	10.69
Onshore “up-to-date” 40% $P_{in,max}$	1.36	0.17	5.23	5.96	0.79	0.34	0.01	7.90	8.63
Onshore “up-to-date” 60% $P_{in,max}$	1.67	0.20	5.12	5.83	0.65	0.42	0.01	8.07	8.78
Onshore “up-to-date” 80% $P_{in,max}$	2.01	0.25	5.01	5.71	0.78	0.50	0.01	8.56	9.26
Onshore “old” 40% $P_{in,max}$	1.96	0.24	2.43	3.14	0.76	0.49	0.01	5.90	6.61
Onshore “old” 60% $P_{in,max}$	2.63	0.32	2.36	3.05	1.02	0.66	0.01	7.00	7.69
Onshore “old” 80% $P_{in,max}$	3.37	0.41	2.30	2.97	1.31	0.84	0.01	8.24	8.91
Offshore 40% $P_{in,max}$	1.18	0.14	8.70	9.44	0.69	0.29	0.01	11.01	11.75
Offshore 60% $P_{in,max}$	1.39	0.17	8.59	9.32	0.81	0.35	0.01	11.33	12.05
Offshore 80% $P_{in,max}$	1.62	0.20	8.49	9.20	0.94	0.40	0.01	11.66	12.38

out of their fixed remuneration period is particularly attractive, even though electrolyzer full load hours are higher with “up-to-date” onshore or offshore wind units. The lowest hydrogen production costs of 4.33 € per kg without or 4.99 € per kg with surcharges were determined for direct electricity procurement from “old” wind energy plants, application of AEL technology and an electrolyzer scaling of 40% of $P_{in,max}$. However, it must be taken into account that these costs are still more than twice as high as the costs for industrial hydrogen supply via conventional SMR, which are currently as low as up to 1.5 € per kg and are primarily dependent on the price of natural gas [11].

One application that already appears promising from an economic point of view is to supply the transport sector or hydrogen filling stations, which currently charge 9.5 € per kg [40]. With reference to the standard for hydrogen filling stations introduced by the H2 Mobility Initiative, a direct electricity supply from the onshore wind farms under consideration would be sufficient to cover the hydrogen demand of one or two type L hydrogen filling stations (daily average: 125 refueling processes, 700 kg_{H2}), provided that sufficient hydrogen storage capacity is available. The PV park and the corresponding electrolyzer scaled to 80% of $P_{in,max}$, on the other hand, would have to have approximately four times its considered nominal load to supply one type XS hydrogen filling station (daily average: 10 refueling processes, 56 kg_{H2}) [41].

Direct electricity purchase from offshore wind farms is considered advantageous, since relatively high electrolyzer full load hours can be achieved. This work shows that the electrolyzer utilization rate is highest in this case, however, the hydrogen production costs are also by far the highest with

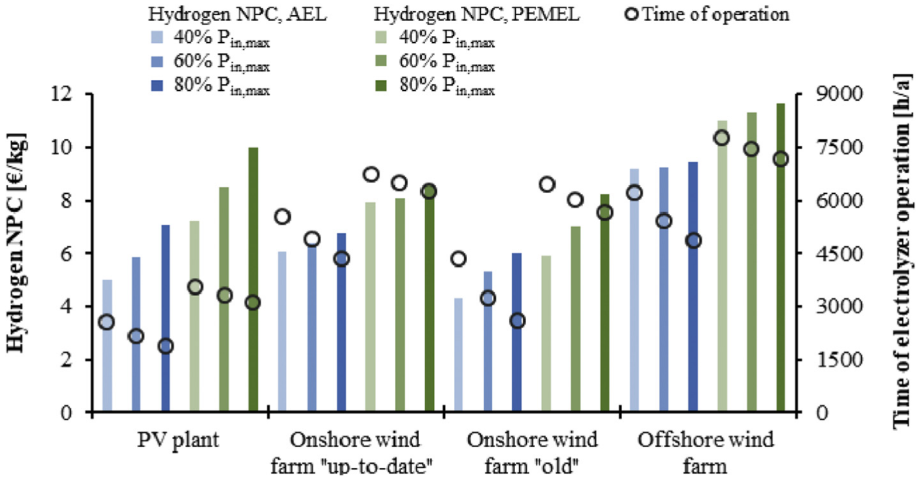

Fig. 10 – Hydrogen net production costs for electricity procurement without surcharges and time of electrolyzer operation.

9.17–12.38 € per kg, since electricity procurement is most expensive.

The techno-economic analysis based on the dynamic operating behavior provides a clear gain in knowledge. Among other aspects, it is shown that stack replacements must be considered depending on actual operating hours. As discussed in the previous subsection, PEMEL may be able to produce more hydrogen than AEL especially with “old” renewable electricity units (PV and onshore wind “old”), but this also associates with longer operating hours and thus at the expense of higher stack costs.

Conclusions

This work reveals that key performance indicators (KPI) such as hydrogen production efficiency, electricity utilization rate, product output and net production costs are highly reliant on the shape of transient power input signals as well as an electrolyzers ability to cope with them.

According to the state of the art, AEL technology is preferable from an economic point of view for electrolyzer operation with a direct renewable electricity supply. The relevance of stack overhaul costs in dynamic operation is striking, which are generally higher for PEMEL. This is due to a shorter stack overhaul period and higher cost per replacement in conjunction with higher operating hours. If, on the other hand, the focus is on the mere utilization of renewable electricity, PEMEL offers advantages. However, due to the higher calculated efficiency for the AEL technology, these advantages do not necessarily result in higher hydrogen production quantities.

It should be noted that the calculated hydrogen NPC are between 4.33 and 12.38 € per kg and are therefore not competitive with industrial hydrogen production from fossil resources. The lowest hydrogen NPC of 4.33 € per kg can be achieved with the onshore wind farm “old” and AEL, although the electrolyzer FLH are limited. This is due to low electricity procurement costs. It further demonstrates that the cheaper purchase of onshore wind power outweighs the higher FLH of offshore wind power. This trend may change in the future, as a significant cost degradation is expected for the provision of offshore wind energy.

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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.

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Nomenclature

Symbol	Parameter	Unit
α	Charge transfer coefficient	-
b_{KOH}	Molality of the potassium hydroxide electrolyte	mol/kg
ΔE_0	Reversible cell potential	V
ΔG	Gibbs free energy	J/mol
ΔH_i^0	Standard enthalpy of component i	J/mol
ΔS_i^0	Standard entropy of component i	J/(K·mol)
δ_{el}^j	Thickness of electrode j	m
δ_{sep}	Thickness of separator	m
δ_{mem}	Thickness of membrane	m
δ_{ccoll}^j	Thickness of current collector of electrode j	m
ε_{sep}	Porosity of separator	-
η	Overpotential	V
η_{act}^j	Activation overpotential of electrode j	V
$\eta_{\Omega,el}^j$	Ohmic overpotential of electrode j	V
$\eta_{\Omega,sep}$	Ohmic overpotential of separator	V
η_Ω	Ohmic overpotential	V
Θ^j	Bubble coverage of electrode j	-
ρ_{sep}	Resistivity of separator	Ohm·m
σ_{ccoll}^j	Conductivity of current collector of electrode j	S/m
σ_{mem}	Conductivity of membrane	S/m
$\sigma_{KOH,free}$	Conductivity of bubble free electrolyte	S/m
τ_{sep}	Tortuosity	-
τ_t	Time constant	-
γ^j	Rugosity of electrode j	m^2/m^2
ω_{sep}	Wetability factor	-
A_{Cell}	Cell area	m^2
$A_{hx}H_{hx}$	Product of heat exchanger area and heat transfer coefficient	K/W
A_{el}^j	Area of electrode j	m^2
A_{p-enh}^j	Factor for pressure enhancement	$(bar\cdot;m^2)/A$
C_c	Heat capacity of cooling water	J/K
C_t	Heat capacity of stack	J/K
c_{p_c}	Specific heat capacity of the heat transfer medium	J/K/kg
c_{p,H_2O}	Specific heat capacity of (liquid) water	J/K/kg
E_{act}^j	Activation energy of electrode j	J/mol
F	Faraday constant	sA/mol
I	Current	A
i_0^j	Exchange current density of electrode reaction j	A/m^2
i_{cell}	Current density	A/m^2
$i_{0,ref}^j$	Reference exchange current density of electrode reaction j	A/m^2
j	Anodic or cathodic cell compartment	-
k_0^j	Electrode rate parameter	mol/Ksm^2
K_{el}	Electricity costs	€/Wh
K_{H2O}	Water costs	€/m^3
K_R	Replacement costs	€/(a·W)
K_{SaM}	Service and maintenance costs	€/(a·W)
K_{TaI}	Taxes and insurance costs	1/a

— (continued)

Symbol	Parameter	Unit
l^{j}_{sep-el}	Distance between separator and electrode	m
$\dot{m}_c$	Mass flow of cooling water	kg/s
N	Number of cells	-
$\dot{n}_i$	Molar flow of species i	mol/s
p_0	Reference pressure (1 atm)	Pa
p_i	Partial pressure of species i	Pa
R	Universal gas constant	J/K/mol
R_Ω	Membrane resistance	Ohm
R_t	Thermal resistance	K/W
P_{act}	Power consumption electrolyzer system	W
P_{aux}	Peripheral power consumption	W
P_{diff}	Available power input to stack	W
P_{ely}	Power of electrolyte pumping	W
P_{grad}	Maximum permitted power gradients	W
P_{grid}	Unutilized power	W
P_{in}	Power input	W
$P_{in,max}$	Maximum power input	W
P_N	Nominal load	W
P_{pmp}	Power of pumping reactant/cooling water	W
P_{pwr}	Power of power electronics	W
P_{st}	Power consumption stack	W
P_{tsa}	Power of temperature swing adsorption	W
T	Stack temperature	K
T_a	Temperature of ambience	K
T^{i}_{c}	Cooling water inlet temperature	K
U_{cell}	Cell voltage	V
U_{OC}	Open circuit potential	V
U_{tn}	Thermo-neutral voltage	V
W_{el}	Annual electrical work	Wh/a
$\dot{V}_{H2O}$	Annual volumetric water demand	m^3/a
z	Number of electrons exchanged	-

Index of abbreviations

ACAPEX	annualized capital expenditures
AEL	alkaline electrolysis
BoP	balance of plant
CAPEX	capital expenditures
CTRL	Control
EEG	renewable energy law
EnWG	German energy law
FLH	full load hours
GHG	greenhouse gas
HER	hydrogen evolution reaction
IR	interest rate
KOH	potassium hydroxide
KPI	key performance indicators
LHV	lower heating value
NPC	net production costs
OER	oxygen evolution reaction
OH	operating hours
OP	stack overhaul period
OPEX	operational expenditures
PEMEL	polymer electrolyte membrane electrolysis
PID	proportional–integral–derivative
PO	annual product output
PMP	Pump
PV	Photovoltaic
PWR	Power
RF	ratio factor
SL	system lifetime
SMR	steam methane reforming
TEA	techno-economic analysis
TRL	technology readiness level
TSA	temperature swing adsorption

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Chapter VIII

8. From Niche to Market - An Agent-Based Modeling Approach for the Economic Uptake of Electro-Fuels (Power-to-Fuel) in the German Energy System

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From Niche to Market—An Agent-Based Modeling Approach for the Economic Uptake of Electro-Fuels (Power-to-Fuel) in the German Energy System

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Abstract: The transition process towards renewable energy systems is facing challenges in both fluctuating electricity generation of photovoltaic and wind power as well as socio-economic disruptions. With regard to sector integration, solutions need to be developed, especially for the mobility and the industry sector, because their ad hoc electrification and decarbonization seem to be unfeasible. Power-to-fuel (P2F) technologies may contribute to bridge the gap, as renewable energy can be transferred into hydrogen and hydrocarbon-based synthetic fuels. However, the renewable fuels production is far from economically competitive with conventional fuels. With a newly developed agent-based model, potential developments in the German energy markets were simulated for a horizon of 20 years from 2016 to 2035. The model was constructed through a participatory modeling process with relevant actors and stakeholders in the field. Model findings suggest that adjusted regulatory framework conditions (e.g., exemptions from electricity surtaxes, accurate prices for CO_2-certificates, strong start-up subsidies, and drastic emission reduction quotas) are key factors for economically feasible P2F installations and will contribute to its large-scale integration into the German energy system. While plant capacities do not exceed 0.042 GW in a business-as-usual scenarios, the above-mentioned adjustments lead to plant capacities of at least 3.25 GW in 2035 with concurrent reduction in product prices.

Keywords: power-to-fuel; power-to-gas; power-to-liquid; agent-based modeling; synthetic fuels; Energiewende; Germany’s energy transition; European Union emission trading system (EU ETS); Erneuerbare-Energien-Gesetz (EEG) Umlage

1. Introduction

The German Energiewende has been focused on the electricity sector, and 42.1% of electricity came from renewable sources by the end of 2019 [1]. Common assumptions assume that renewable electricity will be the only energy source that might match the overall energy demand sustainably in Germany [2–4]. Biofuels, which currently supply 5% of the mobility sector’s fuel consumption, have a limited sustainability potential due to land use conflicts [5–8]. Since photovoltaic and wind power are intermittent and have low full load hours, large capacities are required to achieve 100% of renewable energy (RE) supply in all sectors and to meet the climate protection goals of the Paris Agreement (COP21) [9,10]. As a consequence, the amount of curtailed excess electricity from wind and solar power has already increased. As of 2017, 5.5 TWh of potential generation could not be fed into the grid due to congestion or mismatched demand. In 2017, 610 million euros had to be compensated by end consumers, most of which are private households, due to legally guaranteed feed-in tariffs [11]. Such developments decrease the acceptance of the Energiewende and cause resistance to the installation of new wind and photovoltaic (PV) power plants.

It will be challenging—if not impossible—to find solutions based on direct use of electricity for energy intensive sectors such as aviation, shipping, and heavy road transport as well as the production of hydrocarbon-based raw materials for industry, especially the chemical sector. Several studies conclude that hydrocarbon-based fuels will remain an essential part of the world's energy supply, even when fossil fuels are completely displaced [12–14]. Power-to-fuel (P2F) technologies might close the gap between renewable electricity generation and final energy demand in the above-mentioned sectors. Based on the splitting of water into hydrogen and oxygen via electrolysis (power-to-hydrogen, $P2H_2$), hydrocarbons can be created from hydrogen and a sustainable carbon source by specific synthesis routes such as Sabatier process and Fischer–Tropsch synthesis (hydrogen-to-fuels) [15–17]. With the supply of synthetic and highly energy dense fuels, the share of renewables in all sectors can be increased.

In Germany, more than thirty pilot plants for the production of hydrogen, methane, and liquid fuels are operating today [18,19]. From a technical perspective, P2F has now attained a high level of technology development. It is ready for up-scaling to the multi-megawatt scale. However, due to disadvantageous legal framing conditions, low efficiencies, and high investment costs, P2F plants are not yet economically feasible. As conventional fuels are available at low prices, there is barely an existing demand for the renewable substitutes only in small niche markets [20].

To explore the possible role of P2F in the energy system transition, we investigated pathways for an economic integration. Our model-based analysis focused on socio-technical and socio-economic relations within the German energy system with the goal of identifying key factors for an economic uptake. Stakeholders and actors were categorized in representative operator and customer groups and implemented as interactive agents within German energy markets. Based on the model, the growth rate of P2F plants in Germany over a time horizon from 2016–2035 was evaluated for different scenarios with individual political, technical, and societal developments. The approach of simulating potential real-world behavior of major energy system actors allows one to identify conditions which may lead to an economic success of P2F.

2. Current State of Affairs of P2F in Germany and Methodological Approach

To fulfill the long term German climate change mitigation targets (greenhouse gas reduction up to 95% compared to 1990) and a near 100% renewable energy supply for all sectors, a decisive role of P2F in de-fossilizing parts of the mobility and the industry sectors is inevitable. Depending on assumptions regarding available space for RE installations, studies estimate a wide span for renewable electricity potential of 462–3939 TWh a^{-1} [3,4]. However, the maximum potential for biofuels is considered to be below 500 TWh a^{-1} [5,21,22] due to the scarcity of appropriate farming land and low energy yield per unit area. The photosynthesis and the area-based efficiencies of biomass are lower than photovoltaic and wind power efficiencies. In addition, there is potential in non-farmable areas such as offshore and rooftops that are not suited or used at present.

In Germany, research efforts with regard to synthetic fuel production at the scale of pilot plants started in 2009. Promoted by different research funds, a wide range of pilot projects are being developed, most of them with a focus on the production of hydrogen and methane. In most cases, the produced gases are injected into the natural gas grid, and the major goal of these plants is to serve as a technical proof of concept and an optimization of flexible production modes.

As projected in many scenarios, P2F will provide large shares of energy to different sectors [23–25]. To reach this goal, an up-scaling of existing concepts will be a next step to investigate its potential for industrial integration. Viable business cases exist for at least two pilot projects [20], where renewable hydrogen is fed into the natural gas grid and sold to private households that have a high willingness to pay. Even though the share of the renewable gas remains below 1% in the offered gas mix, these customers pay for a more sustainable premium quality and support the new technology. However, this is only a small niche market with limited sales volumes.

As the Federal Environment Agency and Müller-Syring et al. state in recent studies, production costs for the synthetic substitutes are significantly higher than prices for fossil fuels and biofuels, with production costs of up to 90 cents kWh^{-1} for synthetic methane compared to 2.5 cents kWh^{-1} for natural gas [14,26,27]. Depending on investment costs and surcharges on electricity prices, high production costs of synthetic fuels are very likely, even at levelized costs of electricity considered to be 0 cents kWh^{-1} and at a high number of full load hours. To achieve economic competitiveness, the following factors are widely discussed in literature to be of major importance:

- Reduction of investment costs
- High conversion efficiencies
- High utilization rates
- Reasonable legal framing conditions

Thus, these factors are considered in the further analysis of this work amongst others to quantitatively assess their impact on an economic uptake.

2.1. *Defining Framing Conditions with the Help of the Turtle Model*

The central goal of this study is to find conditions that allow the P2F concept to grow from a small niche to a substantial part of the energy markets. With respect to future uncertainties about markets and technologies, climate change impacts, and other stressors to the system, it is important to find the most relevant so-called impact factors for energy systems transformation. According to the multi-impulse hypothesis, impacts on the direction of innovation processes may arise from changes in technical, societal, economic, and ecological framing conditions or through unforeseeable incidents [28–30]. Effects on innovation directions and the role of different impact factors can be visualized and qualitatively discussed with the help of the turtle model displayed in Figure 1 [31–37]. In the core of the model, a network of participants in the innovation process is displayed. In the long run, companies from many industries might become part of the P2F innovation network. Today, mostly entrepreneurs and progressive companies are the major actors in this young environment. They started with the installation of the first pilot plants, assisted by research institutes and governmental funds. Furthermore, participating actors formed strategic networks to push the development phase forward and support the introduction of a desirable legislation.

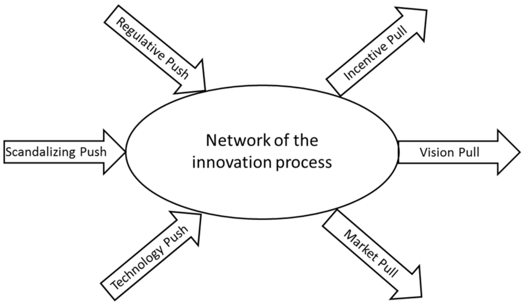


Figure 1. Turtle model—an internal network basically consists of key stakeholders and is accompanied by several external impact factors [31–37].

The six impact factors can be distinguished into push and pull factors. While push factors have the ability to destabilize existing regimes and create new possibilities for innovations, pull factors exhibit a selective effect and promote the innovation direction. In the case of P2F, the technology push is a central driver of the innovation and creates technological options. Further improvement of technologies with regard to efficiency and investment costs is an additional basis for the integration of P2F in the energy markets.

The market pull represents demand for new products, which leads to directed innovation efforts. Currently in niches, there may be a growing demand for synthetic fuels by airlines and transport companies and later on by private households. This demand on the one hand is caused by emission restrictions and on the other hand by ethical preferences which result in a higher willingness to pay for the "green" product.

The regulative push summarizes any governmental regulations which cause changes for the actors' network. Strong impulses might be created by the adoption of new laws. An example is the European Union (EU) regulation on CO_2 emissions of car fleets, which forces car manufacturers to decrease their average fleet emissions [38]. Without such regulative signals, climate friendly innovations can hardly find a way into the markets, giving the regulative push a strong position.

The impact factor incentive pull contains all governmental promotion for pioneers and innovations. Without subsidies, innovations can hardly be developed. Especially in the early development phase, supporting mechanisms such as tax benefits are a common measure to incentivize innovations, e.g., in the case of P2F, operators do not have to pay network use fees (see Section 3). Furthermore, the funding of research projects is a fundamental promotion for new technologies and concepts. Subsidization of P2F projects can be considered as crucial for further market integration.

The scandalizing push is an impact factor that arises from the awareness of the civil society to new developments and old habits. Consumer and environmental protection organizations have the ability to scandalize certain technologies and thereby have an enormous impact on innovations. In contrast to P2F, which, to date, does not seem to face acceptance problems, biofuels were strongly scandalized in Germany (campaign "land use for tank or plate?").

Guiding orientations are represented by the impact factor vision pull, which directs and drives efforts for innovations. With regard to P2F, the development progress is driven by the vision of an environmentally friendly energy system, a high degree of national self-supply leading to more energy independence and a higher national value. Figure 2 summarizes the identified drivers for the P2F innovation system.

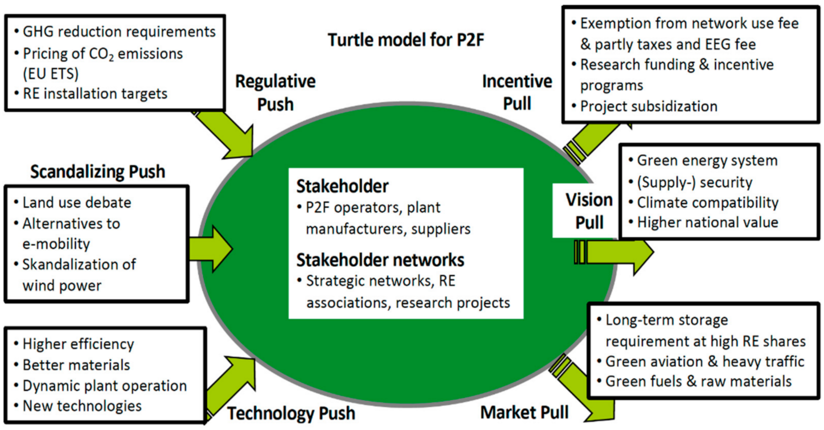


Figure 2. Turtle model for power-to-fuel (P2F)—the turtle model filled with qualitative information on the P2F innovation system gathered from stakeholders, literature review, and policy analysis. Source: authors own compilation.

With the turtle model and its assembly of push and pull factors, the main drivers of the innovation process can be visualized and qualitatively interconnected. However, more complex interrelations between actors and their environment are not included, and a dynamic investigation of how the innovation system may develop over time is not possible within this approach. For a dynamic and quantitative analysis, we used this model as the basis for a newly developed agent-based model (ABM) and evaluated the quantitative impact of each impact factor of the turtle's model.

2.2. Conceptualization of the Agent-Based Model

The ABM was set up using the method of van Dam et al. to analyze framing conditions, which are desirable for a profitable operation of P2F plants [39]. Explicitly and in accordance with Section 2.1, the importance of subsidization mechanisms and their impact on private investments as well as social and regulatory impacts besides technology development are the focus of this investigation.

We implemented a deterministic ABM that simulates the situation depicted in Figure 3 by representing the various actors as individual decision-making agents. The energy system is modeled as one single system in which the demand for each energy carrier is subdivided into single markets with their own participants, prices, and sales volumes (see Table 1). The purpose of the model is to study the uptake "from niche to market" of the P2F technology, given the various push and pull factors depicted in Figure 2. The ABM can be used to explore options for cost-effective paths towards this uptake, as seen from the perspective of different stakeholders.

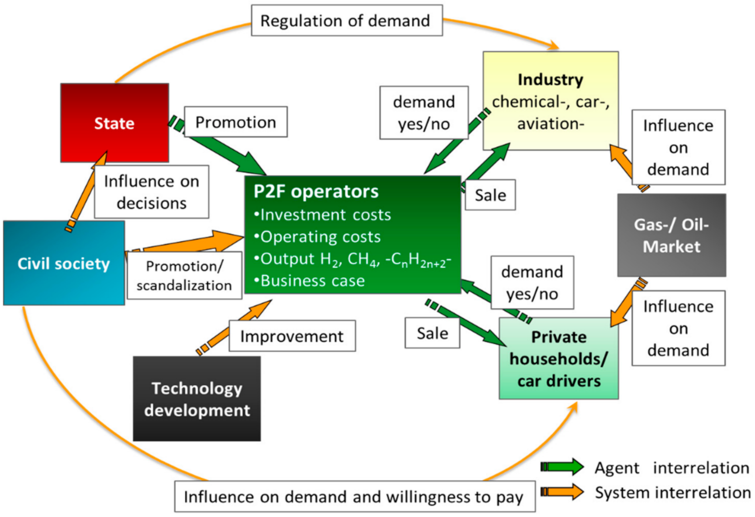


Figure 3. Scheme of the agent-based model's (ABM) conceptualization based on the conversion of the turtle model and van Dam et al. Green arrows indicate direct agent interactions, orange arrows indicate interactions within the system environment (between impact factors). Source: authors own compilation.

Table 1. Demand volume in subdivided markets and assigned market prices in 2015 for Germany based on [40–44].

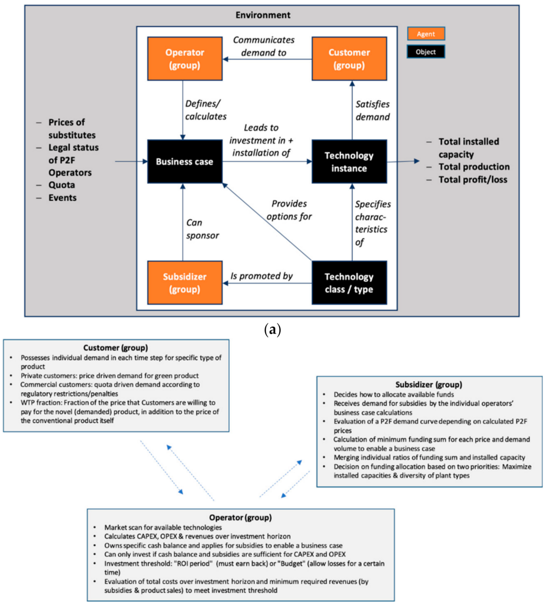
Energy Carrier in Markets	Demand in TWh a^{-1}	Energy Carrier in Markets	Price in € kWh^{-1}
Natural Gas		Natural Gas	
Private households	289	Private households	0.072
Industry	225	Industry	0.036
Transport	2.47		
		Mineral Oil	0.073
Hydrogen			
Industry	60	Biofuels	
Traffic	0.025 (Own assumptions based on registered fuel cell vehicles in Germany. Assumed fuel consumption: 1 kg_{H2} per 100 km. At 15,000 km a^{-1} the total consumption equals 25 GWh a^{-1}.)	Gas	0.08
		Diesel	0.078
Mineral Oil		Petrol	0.07
Industry	36		
Transport	681	Hydrogen	
Households	157	Industry	0.06 (Own calculation of production costs for H_2 via steam methane reformation at a gas price of 3 ct kWh^{-1}.)
		Transport	0.28 (Price information of Clean Energy Partnership (CEP).)

The model revolves around investment decisions made by a variety of P2F operators and purchasing decisions made by customers, all within a dynamic context of evolving regulation and technological progress. The regulatory push and the incentive pull are represented by the state as an agent in the model. The state sets greenhouse gas (GHG) mitigation requirements and provides targeted subsidies (or does not!). Especially in the early adoption phase, the state is a key driver for the innovation process. Subsidizing mechanisms sponsored by the state help enable the development of uneconomical pilot projects, thereby supporting early technical and economical uptake of the technology. The scandalizing push and the vision pull are represented by civil society and basically influence the willingness to pay of households. For technology push, we implemented technological improvement, resulting in a linearly improving efficiency and decreasing investment costs appropriate to the global capacity growth. Finally, the market pull is represented by private and commercial customer groups that have various motivations for purchasing P2F products. As we learned from current market situations, synthetic fuels can, to some extent, be sold in small niches to private households at premium prices. According to the rational choice theory, especially business companies will most likely not invest in more expensive energy products if they do not experience a benefit [45]. Business customers will have a quota-driven demand, which is strongly dependent on regulatory conditions with regard to GHG reduction efforts. As customer agents, we used private households and car drivers, including hydrogen mobility, as well as industrial sectors (see all agents listed in Appendix A).

The conceptual description above illustrates why ABM is an appropriate tool for our research question. Technology uptake is (or can be) a self-reinforcing process with many interdependencies that can only be understood in an integral way and subjected to a wide variety of potential circumstances when put into a simulation model. The P2F innovation system clearly involves heterogeneity among suppliers as well as buyers of P2F technology and products. In addition, this heterogeneity is essential when looking for high-potential niches for the uptake of P2F. ABM allows a natural way to characterize multiple groups as individual agents interacting in the model, while all agents still have to operate in the same technical, economic, and political context. Finally, the model results are very much oriented towards stakeholders in "the field" and policy. It is important to be able to discuss the concept behind the model and show model results without requiring too much modeling experience. ABM allows communication about the model in an intuitive way—each agent has a goal, a set of characteristics and preferences, and some available actions to achieve this goal. This is usually easier to grasp (than, for example, systems of differential equations). Not only does it make the model easier to communicate, in addition, it helps with validation and enhances trust in the accuracy and the adequacy of the model.

2.3. General Model Description

The Entity Relation Diagram depicted in Figure 4a provides a more technical view of the model structure. The model includes operators, customers, and subsidizers as active agent types, displayed in Figure 4b. Each agent actually represents a whole group of agents who together are considered as individuals. In addition, the model includes technology classes, (installed) technology instances, and business cases as passive object types. Finally, the environment provides the regulatory and the economic context for the interaction of agents and objects. All agents and objects are characterized in Appendix A. The market volume and prices for specific customer groups and energy carriers are listed in Table 1. The overall setup of the model was discussed with stakeholders from the field for validation purposes. The participating stakeholders are leading representatives of companies that operate their own demonstration plants, potential customers, strategic networks, and institutes of transition research.



(a)

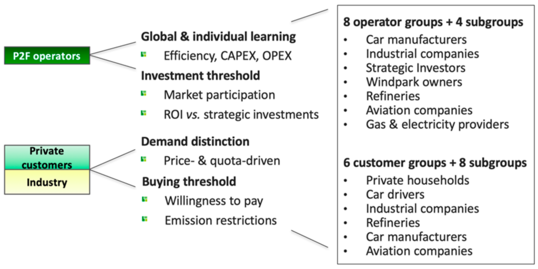
Customer (group)
- Possesses individual demand in each time step for specific type of product
- Private customers: price driven demand for green product
- Commercial customers: quota driven demand according to regulatory restrictions/penalties
- WTP fraction: Fraction of the price that Customers are willing to pay for the novel (demanded) product, in addition to the price of the conventional product itself

Subsidizer (group)
- Decides how to allocate available funds
- Receives demand for subsidies by the individual operators' business case calculations
- Evaluation of a P2F demand curve depending on calculated P2F prices
- Calculation of minimum funding sum for each price and demand volume to enable a business case
- Merging individual ratios of funding sum and installed capacity
- Decision on funding allocation based on two priorities: Maximize installed capacities & diversity of plant types

Operator (group)
- Market scan for available technologies
- Calculates CAPEX, OPEX & revenues over investment horizon
- Owns specific cash balance and applies for subsidies to enable a business case
- Can only invest if cash balance and subsidies are sufficient for CAPEX and OPEX
- Investment threshold: "ROI period" (must earn back) or "Budget" (allow losses for a certain time)
- Evaluation of total costs over investment horizon and minimum required revenues (by subsidies & product sales) to meet investment threshold

(b)

Figure 4. *Cont.*



(**c**)

Figure 4. Overview of the model structure and agent types: (**a**) Entity Relation Diagram; (**b**) depiction of the agent types. All agent types consist of specified groups representing individuals with identical characteristics; (**c**) Overview of operator and customer groups and depiction of their major properties. Source: authors own compilation.

All types of operators, customers, subsidizers, and technology classes that are distinguished in the model as well as qualitative characteristics and initial values of the most important environment variables are stated in Appendix A. In addition, Figure 4c provides an overview of operator and customer groups and their major properties. Complete details about the state variables of each agent and object type as well as the environment are described in the ODD (Overview, Design concepts, Details) protocol [46]. Furthermore, it provides the exact parameterization of all types of agents, objects, and the environment.

Customer agents are heterogeneous with respect to price and volume of demand, according to Appendix A. Price driven agents represent private customers with a higher willingness to pay compared to conventional fuels, motivated by the green quality of the P2F product. At each time step, they are able to decide whether to buy a P2F product or not. Once a P2F product is available on the market within an accepted price range of a customer agent, it buys it. Quota driven agents represent commercial customers that are directly affected by climate protection policies and are enforced to reduce their GHG emissions. In total, they compare the costs of fossil energy plus related charges for GHG emissions with the costs for P2F products. At each time step, they are able to decide whether to purchase the conventional or the P2F product. The individual customer demand volumes are divided into the categories “very small” (≤2% of total demand of this customer group), “small” (≤6%), “medium” (≤15%), and “large” (>15%) (see Appendix A).

Operator agents aim to maximize their installations. At each time step (one step = 1 year), these agents scan the market for available technologies. Depending on their allocated customers and/or the markets they aim to participate in, they choose whether to produce hydrogen (P2H$_2$), methane (P2M), or liquid fuels (P2L). To be able to invest, they possess a specified starting capital and a yearly budget for operation. The capital was categorized as “small” (≤3 million euros), “medium” (≤15 million euros), and “large” (>15 million euros) (see Appendix A). Operating costs are divided into fixed (maintenance, salary, interest, etc.) and variable costs for input electricity and required CO$_2$. Operators are able to achieve learning credits in case they own multiple plants, reducing their fixed operating costs. In addition, operators own an individual investment threshold related to the advanced rational choice theory [40]. Basically, the investment is differentiated by the motivation behind it—is it a strategic investment that may not be profitable from the very beginning but serves as market exploration? An early market integration might be desirable to develop early know-how and yield for a strong position in the new market (early adopters). On the other hand, more conservative operators and investors require profitable business cases with a return on investment within a defined period of time and are not willing to accept structural losses.

While regulatory changes are controlled on the system level, subsidies are provided by the state as an active agent. The amount of the total funding is a variable in the scenarios. The motivation for this agent is to maximize the global installed capacity for all technology classes. Further information on allocation mechanisms is explained in detail in [46].

P2F plants were characterized based on literature [26,47–55]. In the model, these plants were implemented as black boxes based on their current and projected characteristics concerning efficiency, investment, and operating costs. Technical details are considered out of scope. The plants have a utilization rate determining the assigned number of full load hours. It is further assumed that enough renewable electricity and CO_2 will be available at times of operation. According to Sterner et al. and Fürstenwerth et al., efficiencies of the technology classes are assumed to increase linearly by 1% per year [12,56]. However, once a plant is installed, its efficiency remains constant. Investment costs for new installations decrease, as displayed in Equation (1) [57,58]:

$$I_{p(n)} = I_{p(0)} * \left(\frac{p(n)}{p(0)}\right)^{\frac{\ln(0.8)}{\ln(2)}} \tag{1}$$

with $I_{P(n)}$ as investment in year n, $I_{P(0)}$ as investment at the base year, $p(n)$ as capacity in year n, and $p(0)$ as capacity in the basis year.

Finally, the economic and the regulatory contexts were derived from market information in Table 1 and legal aspects discussed in Section 3.

Looking at the model from a farther distance, we can position the model relative to other ABMs by discussing the most distinctive design concepts. One of such concepts is that the model is completely deterministic. Given a certain set of input parameters, agents will always make the exact same choices. In addition, uptake of P2F technology will always follow the exact same pattern. This has obvious performance advantages; there is no need to run a 10,000 iterations Monte Carlo experiment, afterwards trying to make sense of the distributed outcomes. Instead, those 10,000 iterations can be used to explore 10,000 different situations (i.e., combinations of input parameters). The disadvantage of this approach is that the model presumes to always know exactly what choice any stakeholder would make in a given situation. In reality, such choices can at best be seen as stochastic events.

Another distinctive concept is the heterogeneous approach to investment and purchasing decisions. Some operators are willing to make an initial loss on their investment, and some are not. Some have a preference for certain technologies, and others do not. Some customers are incentivized by wanting to be green, and others are forced by regulation. Some buy one product type, while others have multiple options. There is no specific prototype agent from some theory that generalizes all operators or all customers. Instead, we made an effort to do justice to the variation in considerations playing a role in the P2F innovation system based on discussions with stakeholders in the field.

Finally, there is a lot of interaction at the same time, including price developments, technological improvement (conditional on installed capacity), and global and individual learning effects with regard to installation and operating costs. The model does not look at one effect in isolation (although it would allow for such an exercise) but plays out all interactions as a whole.

3. Scenario Description with Consideration of Potential Markets and Legal Aspects for P2F

The economic potential of synthetic fuels is strongly dependent on the conditions of different energy markets for heat, industry, and mobility.

The existing natural gas infrastructure supplies large storage capacities for synthetic gas, and not all heating applications may be covered by power-to-heat or other alternative concepts [59]. However, even though first business cases were realized in niches of the heat sector, it is not expected to become a major market for P2F in the near future. The renewable hydrogen and methane still have to compete with natural gas, which currently is a cheap energy source with prices well below 3 ct kWh^{-1} in 2017 [60] and is predicted to remain so in the near future with prices below 4 ct kWh^{-1} [19].

As another option, the provision of basic chemicals for industries, e.g., ammonia and methanol as well as “green” hydrogen, might become an attractive future market. However, thus far, there are no climate protection restrictions implemented in this market. In the absence of other incentives, industrial companies will not use synthetic substitutes beyond niche applications as long as these come at higher expenses than fossil fuels. CO_2 certificate prices of about 7 € t^{-1} CO_{2eq} until the beginning of 2018 did not appear to have any effect on emission savings in the industry sector [61,62]. Instead, a much higher certificate price for CO_2 emission allowances in the EU emission trading system (EU ETS) on an international basis as well as other GHG emission restrictions might lead to a higher attractiveness of P2F [63]. Reforms to the EU ETS in the recent past have seen an increase in certificate prices from 5.8 € in 2017 to 15.5 € in 2018 [64] and up to 23.40 € at March 2020 [65]. With the approved introduction of an additional carbon tax in Germany from 2021 onwards [66], emission trading is expected to see further price increases within the decade.

Parts of the mobility sector might become the first economically viable applications for synthetic fuels. A broad range of greenhouse gas emission reduction policies is already established and will be enhanced over time. Germany will have to lower its transportation based emissions by at least 38% compared to 2005 according to the effort sharing regulation until 2035 [8]. Currently, biofuels are the most important renewable energy source in the mobility sector to fulfill the GHG emission quota. With regard to this, refineries are facing two dilemmas. (1) Biofuels are barely accepted by society so that petrol and diesel with a higher mix of biofuel can hardly be sold at gas stations, even though they are offered at a cheaper price compared to conventional fuel [67]. (2) In the current legal framework, the renewable share of the total fuel production must increase linearly over time, and the GHG reduction potential of the utilized biofuels must improve as well. P2F might become an attractive alternative for refineries to meet the quota. Furthermore, P2F becoming competitive with biofuels seems more realistic than with conventional fuels.

As car producers must reduce their average fleet emissions to 95 g_{CO_2} km^{-1} in 2020 [68–70], P2F might also become an opportunity to meet these emission restrictions. For this reason, the current largest operating power-to-gas plant in Germany is operated by a big car manufacturer. For the shipping and the aviation industries, there are no emission reduction quotas applied yet. However, the International Air Transport Association (IATA) has set up its own emission reduction targets with CO_2 neutral growth from 2020 on and a halving of the global fleet's overall CO_2 emissions quantities by 2050 relative to 2005 levels [71,72]. Even though first attempts are heading in the direction of biofuels, it cannot be expected that long-term emission reductions will be possible without P2F in the aviation business [73].

3.1. Legal Aspects

Looking at P2F from a life cycle perspective, GHG savings are possible in the fuel production process. In Germany, the former biofuel quota was replaced with a new GHG reduction quota related to the European Fuel Quality Directive (FQD). By adding biofuels as drop-in to conventional fuels, the quota can be fulfilled. While the GHG reduction potential was set to at least 35% compared to conventional fuels until 2017, it has been further increased to at least 50% from 2018 on and up to 60% for plants in operation since October 2015 [74]. For the substitution of conventional diesel, mostly biodiesel is used in Europe today, with about 75% produced from rapeseed methyl ester. However, its GHG reduction potential is calculated to be as low as 37% [75,76]. If the GHG reduction quota is missed, a penalty of 470 € t^{-1} CO_{2eq} needs to be compensated from actors delivering the fuels to the market, e.g., refineries [77].

While legal considerations of synthetic fuels are still to come, restrictions on conventional biofuels are becoming more stringent in the foreseeable future. With an increasingly shifted focus on second and third generation biofuels, the status of synthetic fuels might change towards greater importance [8]. Within Germany, energy storage concepts such as P2F are regulated by the Erneuerbare-Energien-Gesetz (EEG) and the Energiewirtschaftsgesetz (EnWG). Hydrogen and methane are considered as biogas if at least 80% of the utilized electricity originates from a renewable source with a direct connection to the production facility (§ 3 Nr. 10c EnWG). This gives P2F plants a feed-in-priority into the natural gas grid [78]. With regard to additional charges on the levelized costs of electricity, there is an ongoing debate on how to classify P2F plants in the EnWG. At current conditions, P2F plants are considered as an end consumer, resulting in the responsibility of paying several additional taxes and fees [78,79]. As an end consumer, P2F plants are legally treated as private households. Based on the year 2015, and without assuming any exemptions, this results in additional expenses of 22.69 cents per kWh. However, P2F plants are exempt from network use fees (Netzentgelte) for 20 years, even if the output product is not used for electricity generation (§ 118 Abs. 6 Satz 3 EnWG). Furthermore, electrolyzers are exempt from electricity tax (Stromsteuergesetz, StromStG § 9a Nr. 1). Besides these reductions, additional charges of 13.06 cents per kWh still remain. The biggest part of the remaining charges is the EEG fee of 6.405 cents per kWh as it was in 2019 [80]. For the future, stakeholders in the field of P2F expect and demand major changes in the legal framework. Beginning with the National Hydrogen Strategy, several ministries enforce the production of hydrogen, and new funding is approved. It seems likely that legal framing conditions will soon become more favorable for the production of green hydrogen and synthetic fuels.

3.2. Description of Scenarios

With regard to the discussion in Sections 2 and 3 concerning suitable markets for P2F products, the legal framework, and the actor specific interests, we created three scenarios to investigate possible P2F capacity expansions in the German energy system.

First, model calibration and validation were carried out referring to the actual German development of P2F capacity from 2011 until 2016. Capacity growth was calibrated based on available data for P2F technologies, demand volumes, willingness to pay, market prices, investment thresholds, and allocated funding sums (see Appendix A). We also used this setup for a base scenario with a simulation horizon until 2029. In the base scenario, all framing conditions remain constant to investigate the scale of P2F integration in the close future if no further supporting policies and climate protection directives are applied legally.

Secondly, a moderate policy scenario was developed to simulate the impact of single changes in the framing conditions. In this scenario, a linear rise in market prices for natural gas and mineral oil is implemented, and synthetic fuels are further legally accepted as biofuels by national law (BImSchG). This enables fuel producers (e.g., refineries) to make use of synthetic fuels for GHG mitigation and GHG emission reduction quota fulfillment. In addition, it may influence the investment behavior of car manufacturers and aviation and shipping industries. The simulations run for a time period between 2016 and 2035.

In a third scenario, "EnergiewendePlus" (EW^{+}), we implement further policy adjustments, which are discussed with regard to an ambitious energy system transformation process in all sectors. An exemption from the EEG fee and a legal high GHG reduction potential for synthetic fuels are implemented in this scenario. Within this scenario, we further implement specific changes: stronger subsidization efforts, higher EU ETS certificate prices, change of acceptance patterns, and GHG reduction restrictions for companies. The resulting effects on capacity growth rate and related investment volumes were investigated step by step.

4. Results and Discussion

In this section, we present the simulation results and discuss them in light of the theoretical framework presented in Sections 2 and 3.

4.1. Model Calibration and Base Scenario

The actual installed P2F capacity in Germany in 2015 was 21 MW producing hydrogen, methane, and liquid fuels [81]. The total number of installations stood at 23 with many of those plants operating with electrolyzer sizes below 500 kW.

Figure 5 shows the simulation results of the model calibration and the base scenario. Within the model calibration, the actual capacity growth until 2016 was successfully simulated with only little deviation from real figures. A total investment volume of 46 million euros and an additional 32 million euros of subsidization lead to a total capacity of 22 MW, consisting of 12 MW for the production of hydrogen, 9 MW for methane, and 1 MW for liquids. The ratio of the end product types is also close to the actual distribution. The largest deviation appears in the capacity of liquid fuel production, which was 150 kW in reality in 2016 and 1 MW in the model. This is a consequence of a model restriction allowing a minimum plant size of 1 MW. Installed plant numbers are lower than the real number, also as a consequence of the minimum plant size restriction.

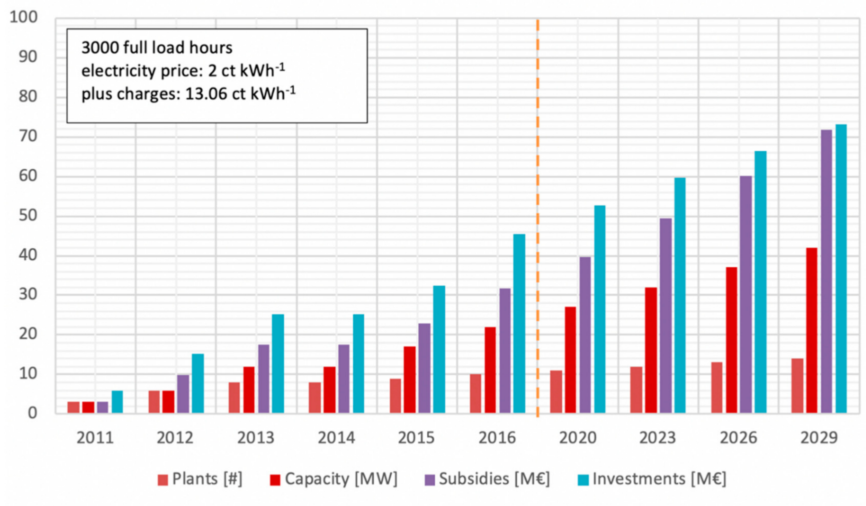


Figure 5. Simulation results of the model calibration and the base scenario (cumulated depiction)—to calibrate the model, the P2F expansion from 2011 to 2016 was successfully simulated. At constant conditions, further capacity growth was simulated until 2029. Source: authors own compilation.

Further simulated development in the base scenario until 2029 shows a total capacity of 42 MW, realized with subsidies of 72 million euros and 73 million euros of private investments. As a result of the slow extension, investment costs barely decreased compared to the start of the simulation. According to Table 2, investment costs for P2H$_2$ installations decreased by less than 14% at the end of the model run compared to 2016. P2M plants achieve a cost reduction of ~12%, while P2L remains constant. The results can be explained by a very limited market volume, which hardly enables business cases. In total, 84 GWh of synthetic fuels are produced in 2029, of which 95% is purchased by private households and only a small fraction of the car industry. As these small markets are increasingly saturated over time, the growth rate is decreasing towards the end of the model run. This is also displayed by the relationship between investments and subsidies, which almost end up in a 1:1 ratio in 2029, since business cases need more funding to be realized. Furthermore, there are no incentives for industrial companies to improve their CO$_2$ balance. Only strategic investors who produce for their own market exploration interests and a small fraction of private households with a willingness to pay of up to plus 20% for the renewable substitute become operators in this scenario.

Table 2. Development of investment and production costs for the different output products in the reference scenario.

	2015		**2029**	
	Investment Costs [€ kW^{-1}]	**Production Costs [ct kWh^{-1}]**	**Investment Costs [€ kW^{-1}]**	**Production Costs [ct kWh^{-1}]**
P2H$_2$	1500	25.7	1292	23.6
P2M	3000	34.0	2630	30.4
P2L	3500	38.7	3500	38.7

P2H$_2$: power-to-hydrogen; P2M: power-to-methane; P2L: power-to-liquid fuels.

Because of high product prices and relatively little demand for P2F products, the production costs hardly decrease as learning effects stagnate. Table 2 shows the modeled production costs in 2015 and 2029, which strongly exceed prices for conventional energy and biofuels.

4.2. Moderate Policy Scenario

Having the model validated, the simulations for the moderate policy scenario start in the model year 2016 and end in 2035. The already preinstalled capacity until 2015 is integrated as starting capacity as well as related subsidies and investments.

As shown in the base scenario, business cases cannot develop with a moderate subsidization being the only supporting mechanism. In the moderate policy scenario, linearly increasing prices for mineral oil and natural gas are implemented, and plant operations at different full load hours are investigated.

- ○ Conventional energy price rise of 2% a^{-1}
- ○ Conventional energy price rise of 4% a^{-1}
- ○ 3000 full load hours in relation to electrolysis capacity
- ○ 6000 full load hours in relation to electrolysis capacity

As energy market price mechanisms are extremely complex, and a forecast for actual price development is not possible, two linear approximations are chosen. The results of Figure 6 show that increasing fossil fuel prices of up to 4% a^{-1} can hardly improve the economic feasibility of P2F plants. Hydrogen and methane production remain the major outputs. The capacity reaches a maximum of 88 MW at 6000 full load hours, which is only slightly above the maximum at 3000 full load hours. The realized projects are still strongly dependent on subsidies and imply a strategic loss-acceptance by progressive operators. Thus, as a result of the economically disadvantageous environment, the installed capacity is lower at 6000 full load hours compared to 3000 full load hours in the 2% a^{-1} price increase case; each operation hour implies a monetary loss as the demand remains too low.

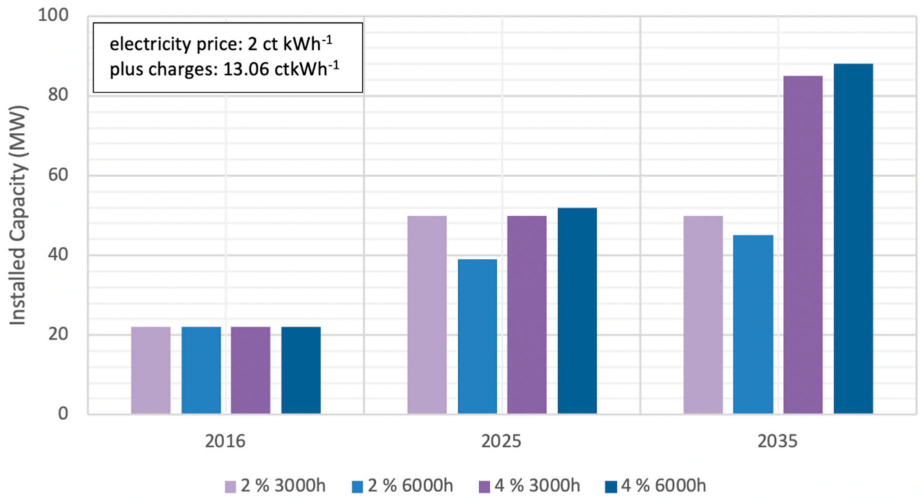


Figure 6. Comparison of capacity development at specific utilization rates and increasing market prices for natural gas and mineral oil.

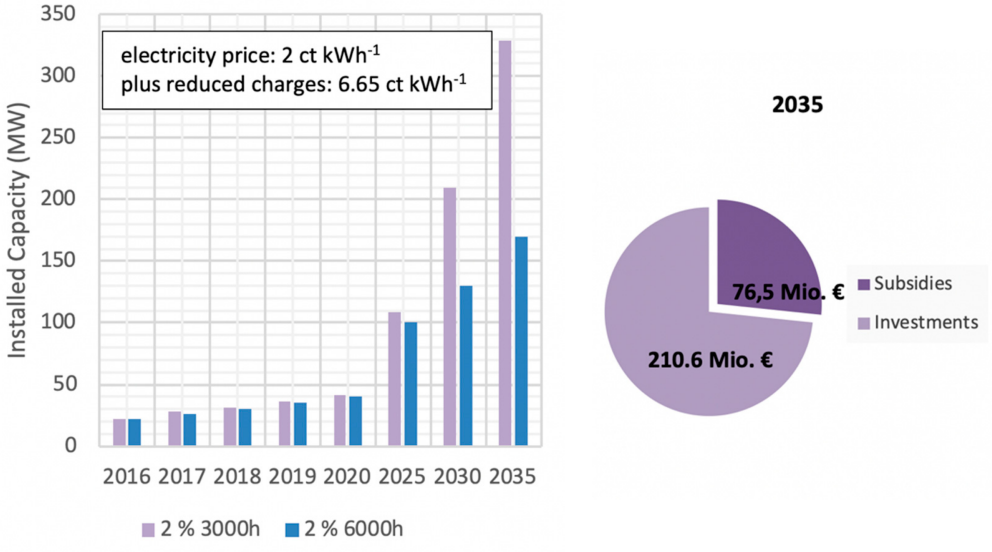
In other words, the fewer hours a plant is running, the more it is economically "feasible", since the operation is always combined with losses. According to Tables 1 and 2, the results are not surprising, since the gap between production costs and market prices cannot be closed by increasing market prices only. The results reveal that regulatory signals are essential for an integration of the P2F technology into the energy system. For industrial companies, there is no motivation to switch from fossil to renewable fuels, as EU ETS certificate prices are low, and only limited restrictions for GHG reduction are realized. At these conditions, the P2F concept will not exceed its current pilot status. A scaling up progress with larger production series and decreasing investment costs will not occur.

4.3. EnergiewendePlus (EW+) Scenario: Optimizing Parameters for an Ambitious Energy System Transformation

4.3.1. EEG—Fee Exemption

A big topic in the general discussion on regulative conditions for operators is the legal status of operators in the Energy Industry Act (EnWG). As stated above, operators are considered as end consumers today. The EEG fee has the biggest share of surcharges on input electricity with 6.354 ct kWh^{-1} in 2016. P2F operators argue that their plants should be considered as a storage or a conversion device in the Energy Industry Act, as the installations do not consume electricity but convert it into storable chemical energy. Without the EEG fee, the surcharges for input electricity reduce from 13.06 ct kWh^{-1} to 6.65 ct kWh^{-1} in the year 2016 (see Appendix A).

Figure 7 shows the capacity development for 3000 and 6000 full load operating hours at moderate increasing fossil energy prices of 2% a^{-1}. As a result of the much lower electricity procurement costs, the capacity grows up to 321 MW in 2035 with 3000 full load hours. With production costs still above 13 ct kWh^{-1} in the case of hydrogen and >18 ct kWh^{-1} for methane, the substitutes remain more expensive than natural gas, mineral oil, and biofuels. This is also indicated by the slower capacity growth at 6000 full load hours. However, the more attractive framing conditions lead to much higher investments in relation to subsidies. A total funding of ~77 million euro activates private investments almost three times higher, which end up in the niche markets, where private households and car drivers pay for the renewable substitutes.

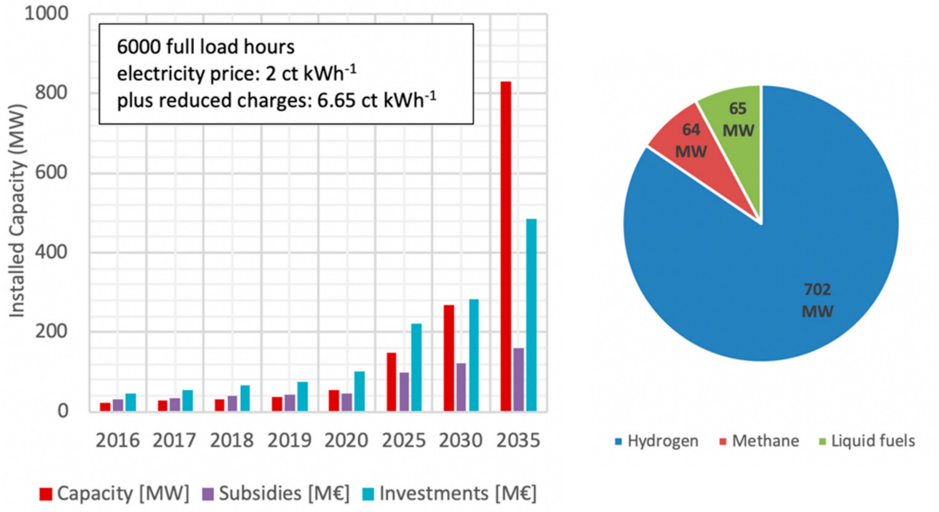


(**a**) (**b**)

Figure 7. Simulation results with EEG-Fee exemption: (**a**) Capacity development with reduced surcharges of 6.65 ct kWh^{-1} (without EEG fee compensation; (**b**) the impact on the ratio of private investments and subsidies. Source: authors own compilation.

4.3.2. Biofuel Recognition

Another discussion point in the P2F network is the legal recognition of synthetic fuels as biofuel. The EU parliament adjusted relevant directives (FQD and RED) in 2015 (and furthermore enacted by the RED II in 2018), which enable customers to legally reduce their GHG emissions by the use of synthetic fuels [82]. As a further extension in the EW$^+$ scenario, the legal recognition of synthetic fuels as biofuel was implemented, which is especially interesting for refineries. The desulphurization process of petrol, diesel, and jet fuel as well as the cracking process of hydrocarbons requires huge hydrogen amounts of ~2.5 TWh per year in Germany [83]. Today, this hydrogen has a fossil energy source, as it is mostly provided through natural gas steam reforming. A substitution by renewable hydrogen could save up to 375,000 tons CO_{2eq} per year. Due to the greenhouse gas reduction quota (Treibhausgasminderungsquote), refineries are obliged to reduce the emissions of their delivered fuels by 6% until 2020. Thus, at desirable framing conditions, synthetic hydrogen might become economically interesting for refineries. In the model, a high electrolysis capacity of 702 MW evolves in 2035 if renewable hydrogen is legally acknowledged as biofuel (see Figure 8).



(**a**) (**b**)

Figure 8. Simulation results with implemented biofuel recognition: (**a**) Capacity development with synthetic fuels being accepted for greenhouse gas (GHG) reduction quota fulfillment; (**b**) $P2H_2$ plants achieve the largest market share with >702 MW in 2035 compared to low capacities for the production of methane and liquids. Source: authors own compilation.

4.3.3. High Willingness-to-Pay

In contrast to biofuels, P2F concepts are not yet confronted with negative acceptance issues. Instead, the opposite seems to be the case, indicated by the willingness-to-pay (WTP) of customers [20]. A special feature of the ABM is the consideration of acceptance patterns. The experiments also include simulations of a high acceptance of synthetic fuels which may result, e.g., from unpredictable extreme events or new scientific insights about consequences of climate change. For such a scenario, it was assumed that up to 10% of private households are willing to pay a premium of plus 15% for green fuels compared to prices of conventional energy providers, and 5% of the households pay a premium of up to 25%. Figure 9 shows the impact on the capacity growth up to 2.7 GW in 2035. Whether considered realistic or not, the results reveal that either a high WTP for renewable products or legally enforced quotas are required besides higher price levels of fossil energy.

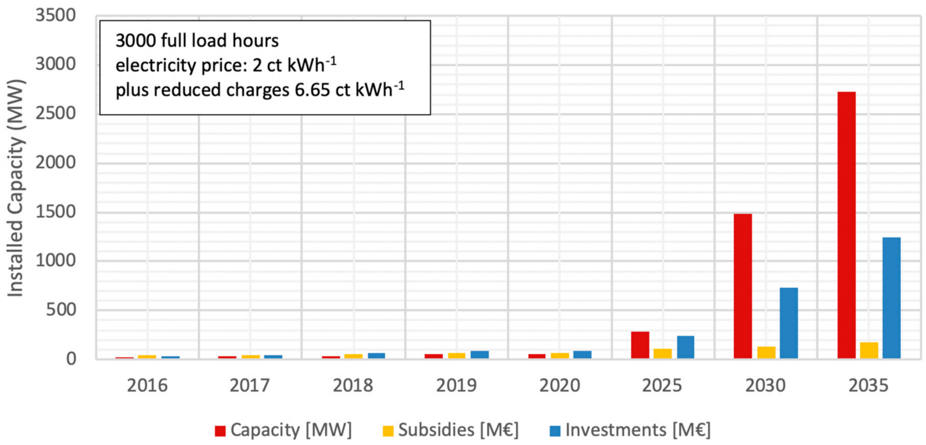


Figure 9. Results assuming a willingness to pay for a premium of plus 15% by 10% and of 25% by 5% of the households for synthetic fuels. Source: authors own compilation.

4.3.4. Strong Legal Regulations

In a last optimization step, such acceptance patterns were not considered. Instead, a scenario with a focus on subsidization mechanisms was created, since all of the above results show a strong dependence on subsidies. For the simulation of an economic integration independent from subsidies in later phases, further adjustments were implemented:

- High EU ETS certificate price of 100 € ton CO_2^{-1} from 2021 on
- Strong start-up subsidization of 60 million € a^{-1} until 2025
- Strong GHG reduction quotas for industrial companies leading to a WTP of up to 30%.

Figure 10 shows that an economic uptake is possible if consequent climate protection measures are realized and research funds for the realization of new projects are strongly increased in the early development phase until 2025.

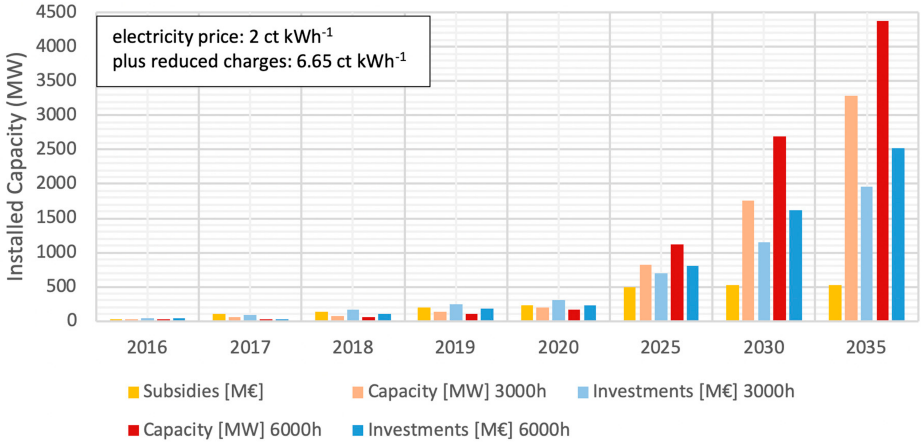


Figure 10. Economic uptake of the P2F technology enabled by strong regulative signals: a high certificate price (100 € per ton CO_2 from 2021), strong subsidization in the early development phase (60 million € per a until 2025 for new projects), and strong emission reduction quotas.

New P2F plants are installed to serve most of the implemented markets with renewable fuels. Figure 10 also indicates that, even though subsidization in the second decade of the model run is stopped, a rapid capacity growth is enabled by private investments, leading to a total capacity of 3.26 GW at 3000 full load hours and 4.4 GW at 6000 full load hours, respectively.

A large $P2H_2$ capacity of 2 GW is supplemented by 1 GW of P2L capacity, indicating that especially transportation and petro-chemical industry sectors develop attractive conditions, whereas P2M remains at a relatively low capacity of only 260 MW. From this, it can be concluded that the substitution of methane for heating applications remains the most challenging market due to comparatively low natural gas prices. The high EU ETS certificate price has a lower impact on the natural gas price due to lower emissions from gas combustion in relation to liquid fuels. Table 3 sums up the development of investment and production costs. It is obvious that synthetic fuel will remain on price levels far above today's energy prices, as production costs can hardly decrease below 13 ct kWh^{-1}, depending on the product.

Table 3. Investment and production cost development of $P2H_2$, P2M, and P2L in the model environment with strong legal regulation conditions.

	2015		**2029**	
	Investment Costs [€ kW^{-1}]	**Production Costs [ct kWh^{-1}]**	**Investment Costs [€ kW^{-1}]**	**Production Costs [ct kWh^{-1}]**
$P2H_2$	1500	25.7	520	12.8
P2M	3000	34.0	1000	15.4
P2L	3500	38.7	1000	15.4

4.4. Discussion of Model Results in Comparison to External Studies

A comparison of the model results with findings of related studies reveals that even the capacity growth in the most optimistic scenario is too low to meet the demand suggested by Sterner et al., Agora Energiewende, or Henning and Palzer (see Figure 11). Sterner et al. created a scenario for 100% renewable energy in the electricity sector and also stated an electrolysis capacity of almost 50 GW already in 2025 and 134 GW in 2050 [56]. Agora Energiewende investigated a P2F demand of max. ~20 GW in 2035, increasing up to max. ~135 GW in 2050, depending on the target of GHG reduction and the level of integration in mobility and chemical industry sectors [12]. Henning and Palzer calculated with a total P2F capacity of nearly 200 GW in 2050 to reduce GHG emissions by 90% compared to 1990 [25].

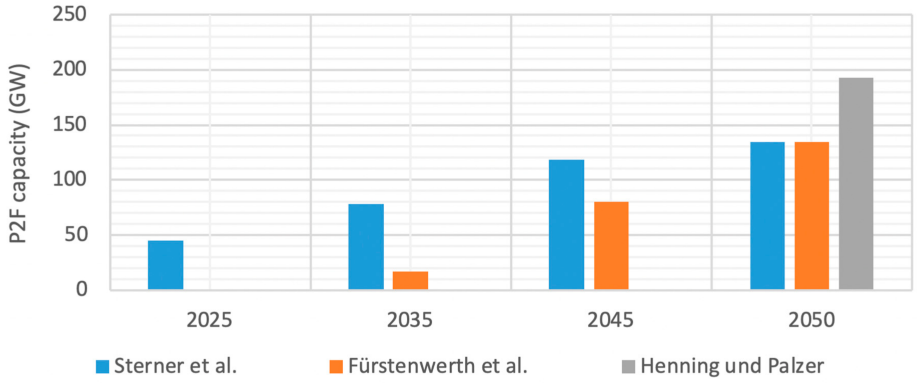


Figure 11. Comparison of capacity estimates in three different external scenarios for an ambitious energy system transformation [12,25,56].

However, the model was developed to find ways out of niche markets in Germany, and possible imports from other countries with lower energy production costs are not considered. Furthermore, once P2F products are economically competitive with fossil fuels, larger investments may most likely occur and may cause a steep rise in capacity development.

5. Conclusions

With a newly developed agent-based model, possible pathways for an economic uptake of the innovation were investigated. Based on today's characteristics and dynamics of the German energy markets and scenarios for future developments, the growth of P2F capacity was investigated within a time period between 2016 and 2035.

The results reveal that consequent regulative adjustments in terms of climate protection and GHG emission reduction in all energy sectors are required for an economic uptake of P2F. Furthermore, high start-up subsidization accelerates capacity growth within the first simulation years and leads to faster price regression and technology improvement. The application of important framework conditions such as EEG fee exemptions, realistic prices for CO_2 certificates, strong start-up subsidies, and drastic emission reduction quotas lead to significant changes in terms of capacity installation and development of product prices. While plant capacities do not exceed 0.042 GW at a base scenario, the above mentioned conditions lead to plant capacities of at least 3.25 GW in 2035. Product prices will decrease concurrently for this case, whereby production costs below 13 ct kWh^{-1} are hard to reach.

While many studies consider large capacities for the production of synthetic hydrogen, methane, and liquid fuels, a clear strategy on how to achieve a large-scale integration is lacking. Stakeholders indicate important aspects which should be considered by policy to allow an economically feasible operation of pilot plants. However, simulations in this study showed that not only single adjustments in the legal framework regarding P2F operation are required. Instead, many different impact factors, especially emission restrictions and the introduction of quotas for renewable fuels in all energy sectors, influence the possibility of an economic uptake.

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Appendix A

Table A1. Overview of crucial model parameters and interacting agents—quantitative values are related to the base year 2015. Capital categorization "small" (≤3 million euros), "medium" (≤15 million euros), and "large" (>15 million euros). Budget categories "very small" (≤2% of total demand of this customer group), "small" (≤6%), "medium" (≤15%) and "large" (>15%).

Operators Operator Group	Customer Base	Techs	Budget/Scale	Investment Criterion
Progressive Car Manufacturers	Mobility	All	Medium	Strategic
Conservative Car Manufacturers	Mobility	All	Large	Profitable
Progressive Industry	Industry	All	Medium	Strategic

Table A1. *Cont.*

Conservative Industry	Industry	All	Large	Profitable
Strategic P2F investor	Broad	All	Medium	Strategic
Wind park operators (big)	Broad	All	Medium	Profitable
Wind park operators (small)	Broad	P2H$_2$/P2M	Small	Profitable
Electricity provider	Broad	P2H$_2$/P2M	Medium	Profitable
Refinery-hydrogen investments	Refineries	P2H	Large	Strategic
Refinery—liquid investments	Refineries	P2L	Medium	Strategic
Progressive gas provider	Households	P2H$_2$/P2M	Medium	Strategic
Conservative gas provider	Households	P2H$_2$/P2M	Large	Profitable
Customers				
Customer Group	**Substitute**	**Product**	**Potential Demand**	**Incentive**
Green households	Hydrogen, methane	Gas	Medium	Willing to pay
Green+ households	Hydrogen, methane	Gas	Very small	Willing to pay
Green car drivers	Methane, liquid fuel	Liquid fuel	Small	Willing to pay
Fuel cell mobility	Hydrogen	Fossil hydrogen	Small	Willing to pay
Green H$_2$ industry	Hydrogen	Fossil hydrogen	Small	Willing to pay
Green gas industry	Hydrogen, methane	Gas	Small	Willing to pay
Green liquid industry	Liquid fuel	Mineral oil	Small	Willing to pay
H$_2$-oriented refineries	Hydrogen	Biofuel	Large	Quota
Liquid-oriented refineries	Liquid fuel	Biofuel	Large	Quota
Gas-based car industry	Methane	Biofuel	Medium	Quota
Liquid-based car industry	Liquid fuel	Biofuel	Medium	Quota
Subsidizer				
Subsidizer Group	**Substitute**	**Subsidy per Year**		
Power-to-hydrogen subsidizer	Hydrogen	3 million euro		
Power-to-methane subsidizer	Methane	3 million euro		
Power-to-liquid subsidizer	Liquid fuel	2 million euro		
Technology Classes				
Technology Class	**Initial Relative Investment Cost**	**Initial Efficiency**	**Pre-Existing (Input) Capacity**	
Power-to-hydrogen	1500 €/kW	65%	12 MW	
Power-to-methane	3000 €/kW	55%	8 MW	
Power-to-liquid	3500 €/kW	50%	1 MW	
Environment				
Environment Variable			**Status**	**Initial Value**
Fixed operating costs in % of investment				4%
Individual relative fixed operating cost reduction per year of experience				2%
Maximum individual relative fixed operating cost reduction				20%
Tax per kWh related to legal status of P2F operators			End Consumer:	0.1306 €/kWh
			Energy-Intensive Industry:	0.0765 €/kWh
			Storage:	0.0665 €/kWh
			Locally produced RE:	0.0254 €/kWh
Legal status of P2F operators			End Consumer	
EU ETS certificate price				6.5 €/ton$_{CO2eq}$
Average utilization of renewable energy plants				22%
Biofuels quota for refineries				6%
Electricity price				0.02 €/kWh

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Chapter IX

9. Mind the Gap - A Socio-Economic Debate on Price Developments of Green Hydrogen, Synthetic Fuels and Conventional Energy Carriers in Germany

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Mind the Gap—A Socio-Economic Analysis on Price Developments of Green Hydrogen, Synthetic Fuels, and Conventional Energy Carriers in Germany

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Abstract: In recent years, the development of energy prices in Germany has been frequently accompanied by criticism and warnings of socio-economic disruptions. Especially with respect to the electricity sector, the debate on increasing energy bills was strongly correlated with the energy system transition. However, whereas fossil fuels have rapidly increased in price recently, renewable substitutes such as green hydrogen and synthetic fuels also enter the markets at comparatively high prices. On the other hand, the present fossil fuel supply is still considered too low-priced by experts because societal greenhouse gas-induced environmental impact costs are not yet compensated. In this study, we investigate the development of the price gap between conventional energy carriers and their renewable substitutes until 2050 as well as a suitable benchmark price, incorporating the societal costs of specific energy carriers. The calculated benchmark prices for natural gas (6.3 ct kWh^{-1}), petrol (9.9 ct kWh^{-1}), and grey hydrogen from steam methane reformation (12 ct kWh^{-1}) are nearly 300% above the actual prices for industry customers in 2020, but below the price peaks of early 2022. In addition, the price gap between conventional fuels and green hydrogen will be completely closed before 2050 for all investigated energy carriers. Furthermore, prognosed future price developments can be considered rather moderate compared to historic and especially to the recent price dynamics in real terms. A gradual implementation of green hydrogen and synthetic fuels next to increasing CO_2 prices, however, may temporarily lead to further increasing expenses for energy, but can achieve lower price levels comparable to those of 2020 in the long term.

Keywords: hydrogen; synthetic fuels; inflation; environmental impact costs

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1. Introduction

On the way to a de-fossilized energy system, the German net electricity production from renewable energy sources already reached 50.3% in 2020 [1]. In contrast, the share of renewable energies in other energy intensive sectors such as transport, heating, and industry remains still low and requires a significant increase according to (inter)national climate protection targets [2]. Besides a direct electrification of applications, green hydrogen from water electrolysis and synthetic fuels from Power-to-Fuel (PtF) processes are considered as important renewable energy carriers in these sectors. Scenarios indicate a national future green hydrogen and synthetic fuel consumption of 250–800 TWh [3]. To satisfy this high demand, large scale production capacities in Germany will be required, complemented by huge import volumes [4]. In line with this, the European Commission published "a hydrogen strategy for a climate-neutral Europe" in 2020, announcing a green hydrogen production target of up to 1 Mt_{H2} a^{-1} until 2024 and above 10 Mt_{H2} a^{-1} in 2030 within the European Union [5]. This strategy is accompanied by the coalition agreement of the German government, targeting an electrolysis capacity of 10 GW_{el} until 2030 in Germany [6].

In Schnuelle et al., it was shown how a national production of green hydrogen and PtF products may enter the market in Germany [7]. With calculated production costs of up to

38.7 ct kWh^{-1} in 2020, these substitutes are considerably more expensive than conventional fuels such as natural gas and crude oil-based products. Other studies show comparable results [8–10]. As a consequence, a substitution of conventional energy carriers by the introduction of green hydrogen and synthetic fuels is suspected to cause rigorous energy price increases. However, a strong scandalization of (increasing) energy prices has already occurred in recent years [11–13]. The recent price jumps since the end of 2021 until today (March 2022) are further inflaming the debate on too-high costs for electricity, natural gas, and crude oil-based fuels.

Whereas the unexpected price developments for natural gas and crude oil already lead to an extraordinary high financial burden for private and commercial customers, the remaining price gap between conventional fuels and renewable substitutes may consequently cause even more intensified price debates. On the other hand, in light of current fossil energy price levels, renewable substitutes suddenly appear rather attractive in the public perception, which indicates a higher acceptance for their rapid rollout. Besides the effects of the current geopolitical tensions, conventional energy carrier prices are also expected to increase further over time. This is especially due to rising emission allowance prices within the European Union Emission Trading System (EU ETS) and newly implemented CO_2 price mechanisms such as the German national Fuel Emissions Trading System (nETS). In this context, other studies analyzed when green hydrogen may reach economic competitiveness compared to fossil fuels under consideration of increasing fossil energy prices and decreasing green hydrogen production costs [14,15]. Aditiya and Aziz discuss the global socio-economic consequences of unstable mineral oil prices within the last few decades and analyze hydrogen integration potentials in the Asia-Pacific region for an enhanced energy price stability [16]. Bleischwitz et al. focused on a transition towards a European hydrogen economy from a socio-economic perspective and evaluated policy framework requirements for a successful implementation of hydrogen technologies in Europe [17]. Maack and Skulason investigated the acceptance of hydrogen applications for its large-scale integration into societal functions [18].

However, an implementation of green hydrogen and synthetic fuels will consequently enforce higher temporal energy price levels. By this means, socio-economic implications are of highest importance in light of potential economic burdens for customers on the one hand and prevention of climate change consequences on the other. Nevertheless, these aspects are usually out of scope in the literature. According to this research gap, two major questions are addressed in this work:

(1) If conventional fuels increase in price and renewable energy carriers also feature high price levels in the future, what should be an adequate benchmark price for both types of energy supply?
(2) To what extent do the recent as well as the expected future price developments lead to an intensified financial burden for customers?

Both questions independently address the dilemma of expectable energy price increases in the short- and medium-term. While energy price related debates are generally highly controversial within (German) society, adequate tradeoffs need to be identified to prevent enormous societal costs in the long-term, besides protecting the (national) economy from short-term energy price disruptions.

With regard to question (1), a focus is set on the environmental impact costs caused by greenhouse gas emissions. Because the production and combustion of any hydrocarbon energy carrier emits specific amounts of greenhouse gases, several studies have carried out a related monetary environmental impact assessment. Under consideration of potential environmental and societal damages as a consequence of climate change, the Federal Environment Agency (FEA) of Germany calculated environmental impact costs of 199 Euro ${t_{CO2eq}}^{-1}$ for the year 2020, which will gradually increase over time. Based on these findings, a suitable benchmark price representing the actual economic costs for natural gas, crude oil, petrol, and grey hydrogen from steam methane reformation (SMR) is examined in Section 2. Furthermore, the price developments of these fossil fuels, as well as for green hydrogen and synthetic fuels, are derived from 2020 until 2050 for private and commercial customers based on a literature review. The price gap between conventional fuels and their renewable substitutes is investigated with and without consideration of greenhouse gas-induced environmental impact costs.

For question (2), a detailed analysis of historic price developments over the past decades, going back to the 1950s, is carried out in Section 3. Projected price trends are compared to former price dynamics in both nominal and real prices. Especially in recent years, the above-mentioned debate on energy prices has continued to heat up. Within this debate, however, inflation effects seem to be widely neglected. Thus, we investigate whether price increases have also occurred in real terms by considering the annual consumer price index development. Furthermore, the expected future price developments until 2050 are set in relation to previous price growth rates as well as to historic inflation-adjusted energy price levels. The findings are finally compared to the evaluated price developments of Section 2, followed by conclusions in Section 4.

2. Price Projections and Consideration of Greenhouse Gas-Induced Environmental Impact Costs

2.1. State-of-the-Art and Prospective Price Developments of Renewable and Conventional Energy Carriers in Germany

Techno-economic analyses on water electrolysis and PtF processes have been carried out by several international studies, such as [19–23]. In a recent study, hydrogen production costs of 25.7 ct kWh^{-1} for 2015 and 12.8 ct kWh^{-1} for 2029 were calculated. Production costs for liquid hydrocarbons from Fischer–Tropsch synthesis were calculated at 38.7 ct kWh^{-1} and 15.4 ct kWh^{-1}, respectively, for the same time horizon [7]. However, a direct coupling to renewable energy facilities such as offshore windfarms was out of the scope of the study. In a further study, detailed green hydrogen production costs in northwest Germany in combination with several renewable electricity production patterns from photovoltaic (PV) and wind power were simulated [24]. Conservative electricity prices as high as the present legal renewable energy act (Erneuerbare Energien Gesetz, EEG) remuneration in Germany for modern onshore wind farms (9.3 ct kWh^{-1}) and offshore wind farms (15.4 ct kWh^{-1}), as well as 4.5 ct kWh^{-1} for old wind and PV farms, were considered. The simulation results revealed levelized costs of hydrogen of at least 13.1 ct kWh^{-1}.

Other studies focused on current and future production costs with direct coupling to offshore wind energy in Germany while taking the actual levelized costs of electricity into account. Rudolph, Pfennig, et al. and Agora Verkehrswende state 19–22 ct kWh^{-1} in 2030 and 13–16 ct kWh^{-1} in 2050 for German synthetic fuel production with offshore wind energy [8,9,25]. Decker et al. state 9.9–18.9 ct kWh^{-1} and 39.3–49.7 ct kWh^{-1} for current offshore hydrogen and methanol production in Germany, respectively [10]. The International Energy Agency (IEA) forecasts green hydrogen production costs of 5–11 ct kWh^{-1} in 2030 at favorable production sites in Europe [26]. Agora Energiewende and Wuppertal Institut project hydrogen predict production costs of 12 ct kWh^{-1} in 2030 and 8.5 ct kWh^{-1} in Germany in 2050 [27]. The International Renewable Energy Agency (IRENA) investigated hydrogen production costs with direct wind or PV power supply. For average wind and PV locations production, costs range from 10.8–17.5 ct kWh^{-1} in 2020, 7.5–8.2 ct kWh^{-1} in 2030, and 3.3–5.0 ct kWh^{-1} in 2050 [28]. These literature-based price ranges for 2020, 2030, and 2050 are applied for further investigations in this study. The respective cost ranges are displayed and linearly interpolated in Figure 1, thus showing best- and worst-case assumptions over the considered time horizon.

In comparison to average conventional hydrogen production costs via SMR as well as to natural gas and crude oil customer prices, the renewable substitutes are only available at rather high production costs. In Europe, hydrogen from SMR production was typically available at costs of approximately 4–6 ct kWh^{-1} in the 2010s, strongly depending on the natural gas price, which accounts for nearly 70% of the total production costs [26]. The latter followed a declining trend for industrial customers in Germany from an intermediate peak of 3.9 ct kWh^{-1} in 2008 to 2.32 ct kWh^{-1} in 2020, excluding VAT. However, since the third quarter of 2021 a rapid multiplication of natural gas prices occurred, with peak spot market prices above 20 ct kWh^{-1} in March 2022 [29]. Natural gas prices for German private households ranged from 5.7–6.9 ct kWh^{-1} between 2012 and the beginning of 2021 and reached 6.2 ct kWh^{-1} by the end of 2020, including all taxes [30]. As a consequence of continual geopolitical instabilities, household prices for natural gas peaked above 16 ct kWh^{-1} at the beginning of 2022 [31]. Due to the tight correlation to natural gas prices, production costs of grey hydrogen increased drastically to 19 ct kWh^{-1} averagely in the first months of 2022 and peaked above 30.19 ct kWh^{-1} [32].

In light of current fossil energy price developments, former developed scenarios and price expectations appear to be rather unrealistic. However, because further price actions in correlation to geopolitical incidences are nearly unpredictable, in this investigation we adhere to the scenarios from the literature. As such, the IEA expects natural gas net prices of 3 ct kWh^{-1} for Europe by 2040 without consideration of increasing CO_2 prices and taxes [33]. Hauser et al. simulated average cross border natural gas prices of up to 5 ct kWh^{-1} by 2050 [34].

Conventional liquid fuel prices strongly correlate with highly fluctuating crude oil import prices. For 2030 and 2050, Kemmler et al. expect crude oil prices of 6.0 ct kWh^{-1} and 6.9 ct kWh^{-1}, respectively [35]. According to Agora Verkehrswende, the price for petrol, excluding taxes, reached 4.7 ct kWh^{-1} in 2020 and is expected to increase to 6.19 ct kWh^{-1} by 2030 and 7.63 ct kWh^{-1} by 2050 [8]. Actual petrol prices in March 2022, however, peaked above 11 ct kWh^{-1} in consequence of the war in Ukraine.

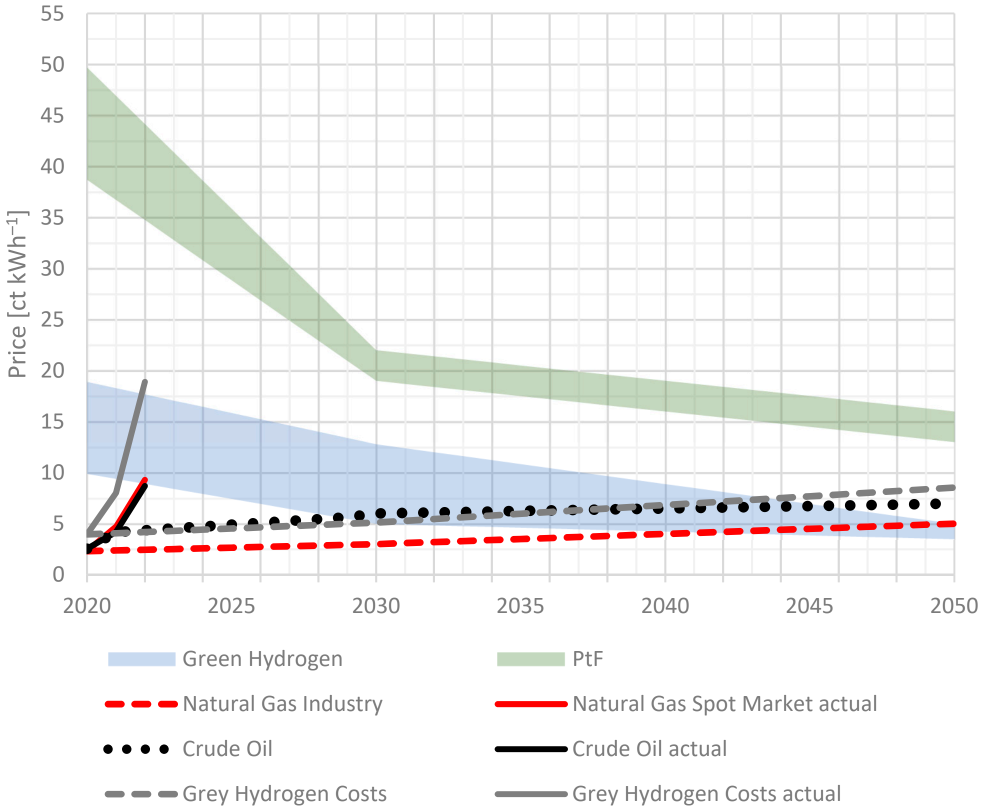


Figure 1. Expected production costs of green hydrogen and synthetic fuels up to 2050 compared to price projections for grey hydrogen, natural gas (prices for industry customers), and crude oil (dashed lines), without consideration of increasing CO_2 emission costs. Prices for grey hydrogen, natural gas, and crude oil in solid lines represent the actual price developments. Linearly interpolated data based on [7–10,24–28,30,33–37].

According to Figure 1, current extreme prices for natural gas and crude oil drastically exceed scenario expectations for the upcoming decades and reach the lower production cost range of green hydrogen in 2022. Nevertheless, the scenario-based expectations for fossil energy carriers also show an increase in price over time compared to 2020. The renewable substitutes instead can achieve declining production costs due to technical improvements and economic upscaling effects among other factors. Investment costs of electrolyzers are expected to reach 200 Euro kW^{-1} once global capacities of 100 GW are realized [28]. Decreasing capital expenditures for electrolyzers and lower levelized costs of electricity from renewable energy sources are considered as key drivers for lower production costs of green hydrogen and synthetic fuels. In consequence and according to Figure 1, the scenario-based price gap of 5.9–14.9 ct kWh^{-1} between green hydrogen and grey hydrogen in 2020 could already shrink to -0.1–7.7 ct kWh^{-1} in 2030 and will be completely closed by 2050. The scenario-based price gap between green hydrogen and natural gas will shrink from 7.65–16.65 ct kWh^{-1} in 2020 to 2–9.8 ct kWh^{-1} in 2030 and could also be closed or even overcompensated by 2050. The production of synthetic fuels instead remains nearly 200% more expensive than the assumed prices for crude oil-based products, even in 2050. Nevertheless, production costs for synthetic fuels in 2050 may almost reach the crude oil prices of March 2022. Green hydrogen can already compete with the early 2022 fossil energy prices.

2.2. Consideration of Greenhouse Gas-Induced Environmental Impact Costs

In the above discussed price comparison, surcharges for CO_2 emissions via specific regulative mechanisms are widely neglected. Besides the European Union Emission Trading System (EU ETS), several additional instruments in the form of carbon taxes and certificates have been discussed or are already implemented. In particular, the newly established German national fuel emission trading system (nEHS) is expected to lift fossil fuel prices in Germany over time. Scenarios expect CO_2 emission prices up to 100 Euro$t_{CO2eq.}{}^{-1}$ by 2050 [26,27]. Surprisingly, allowance certificates within the EU ETS already reached a temporary price of almost 100.00 Euro $t_{CO2eq}{}^{-1}$ in February 2022 [38].

In this work, we do not consider any specific legal CO_2 certificate or tax systems, but rather greenhouse gas-induced environmental impact costs based on investigations of the German Federal Environment Agency (FEA) [39]. Under consideration of socio-economic burdens (e.g., higher expenses for healthcare, crop losses, infrastructure, and building damages) caused by extreme weather events that are related to climate change, the FEA investigated environmental impact costs of 199 Euro $t_{CO2eq}{}^{-1}$ for emissions caused in 2020. This value will increase over time up to 255 Euro $t_{CO2eq}{}^{-1}$ until 2050 and indicates that present energy prices are clearly too low.

Figure 2 displays the above-illustrated price ranges, including the additional environmental impact compensation costs of 0.0199–0.0255 ct $g_{CO2eq}{}^{-1}$. The assumed specific CO_2 emission equivalents for the discussed energy carriers are listed in Table 1. The comparably low values for green hydrogen and synthetic fuels reflect an exclusive utilization of renewable electricity.

Under consideration of the environmental impact costs, a specific benchmark price for each discussed energy carrier can be defined (Table 1). These are calculated based on the 2020 prices for natural gas, grey hydrogen, crude oil, and petrol and on the specific CO_2 emission equivalents shown in Table 1. The benchmark prices represent the actual economic costs of these energy carriers, including expenses for caused environmental and societal damages. Thus, at the latest when green hydrogen and synthetic fuels reach a price level below these benchmark prices, they can be considered beneficial for the national economy. However, in comparison with the energy prices of recent years until the first half of 2021, these price levels are far above conventional energy prices. In contrast, the calculated benchmark prices are well below the energy peak prices of early 2022, which caused dramatic disruptions in the energy markets, economies, and societies concurrently.

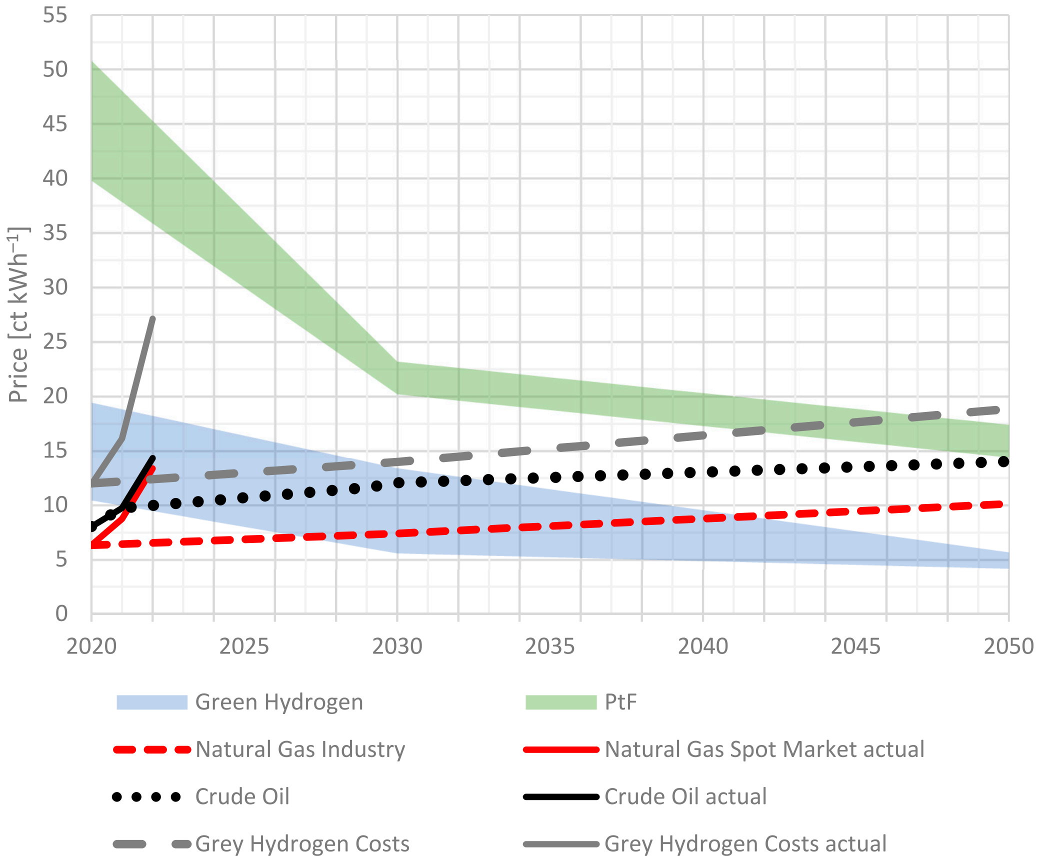


Figure 2. Expected production costs of green hydrogen and synthetic fuels up to 2050 compared to price projections for grey hydrogen, natural gas (prices for industry customers), and crude oil (dashed lines) with consideration of individual environmental impact costs based on [39]. Prices for grey hydrogen, natural gas, and crude oil in solid lines represent the actual price developments including specific environmental impact costs. Linearly interpolated data based on [7–10,24–28,30,33–37].

Table 1. Specific CO_2 equivalents of all considered energy carriers and calculated benchmark prices for conventional fuels. CO_{2eq}. values for green hydrogen and synthetic fuels apply for a production via water electrolysis with renewable input electricity. Values for grey hydrogen apply for a production via steam methane reformation (SMR). Values for specific CO_2 equivalents derived from [40,41].

Energy Carrier	Specific CO_2 Equivalents g kWh^{-1}	Benchmark Price ct$_{2020}$ kWh^{-1}	Price in 2020 ct$_{2020}$ kWh^{-1}
Grey hydrogen	403	12	4
Green hydrogen	26	-	-
Natural gas	200	6.3	2.34
Petrol	275	9.9	4.7
Synthetic fuels	54	-	-

Figure 2 shows a rigorously shrinking and partially even closed price gap between the renewable and fossil energy carriers already today for scenario-based data. While synthetic fuels remain more expensive than fossil fuels until 2050, the price range of green hydrogen partially overlaps with grey hydrogen and crude oil already in 2020. In 2030, the lower price range of green hydrogen is also below the natural gas price. In 2050, green hydrogen is by far the cheapest energy carrier. In comparison to the real price developments and consideration of environmental impact costs, natural gas and crude oil prices range within the production cost range of green hydrogen in 2022.

On the other hand, the average green hydrogen price in 2050 is 200% above the natural gas price in 2020, but cheaper than natural gas in early 2022 and comparable to prices around 2012 (cf. Section 3). Synthetic fuel production costs in 2050 remain up to more than three times higher than the production costs of petrol in 2020. However, the synthetic fuel production costs of 2050 reach a price level comparable to the consumer price of petrol in 2020 (cf. Section 3) and to crude oil prices in 2022.

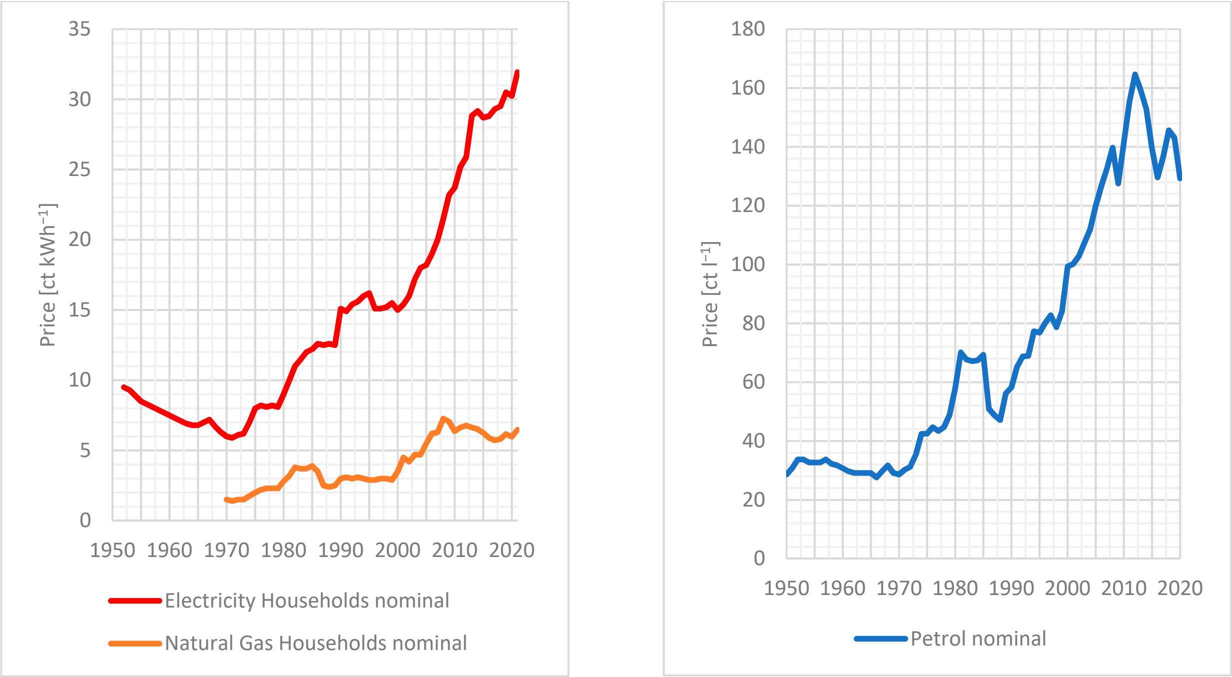
3. Discussion of Price Developments from a Socio-Economic Perspective

Commercial and private customers are apparently confronted with historically high energy prices as a consequence of steep cost increases for fossil energy carriers. Further developments are very hard to predict due to the strong correlation with ongoing geopolitical tensions. This circumstance heavily underpins that the former trust in a supply-secure and reasonably priced fossil-based energy system was rather dicey and urgent transformations are required to ensure both sustainable supply security as well as higher price stability.

Apart from these recent developments, customers also face increasing energy prices according to the findings in Sections 2.1 and 2.2 in comparison with the energy price levels of the last decade. Furthermore, in light of socio-economic long-term costs, the defined benchmark prices indicate that the overall price level of conventionally supplied energy was significantly too low. Even though these results seem to be neither surprising nor avoidable in the context of a sustainability-orientated energy system transition, the question about how societies can handle these monetary challenges is widely open and apparently of paramount importance today. On the one hand, business companies fear (international) economic competitiveness and a loss of their business models. On the other hand, households with low incomes suffer from higher energy costs and struggle with unaffordable energy bills. The current situation shows that both issues need to be addressed with urgent care in energy-related political decisions.

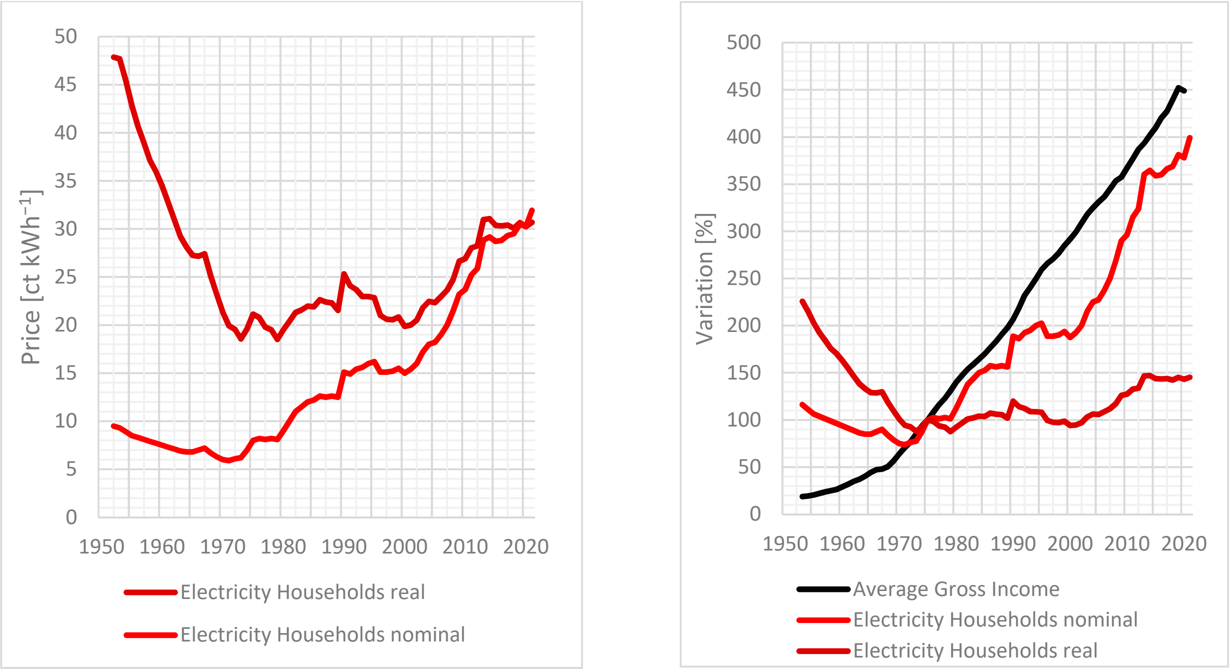
In the context of rising energy prices, however, it is noteworthy that strong fluctuations also occurred in many previous decades, e.g., crude oil price peaks in 1980, 2008, and 2012. A look at historic price charts of natural gas, petrol, and electricity for private households indicates overall increasing nominal prices during previous decades (cf. Figure 3a,b). Public discussions on these developments usually intensified in times of high price growth rates. However, in the context of the German energy system transition, debates on price dynamics have previously flared up before the steep price increases that started in late 2021. Within these scandalizing debates, a special focus was put on the development of the electricity price for end consumers [42–46].

A strong scandalization of the steady nominal price increase of electricity since the early 2000s occurred, and critique was mainly correlated to the subsidization of conventional power plants by wind and photovoltaic energy. In fact, after a long period of stable prices in the 1990s, the average price growth rate from 2001 to 2010 was extraordinarily high at 5.4% a^{-1}. From 2011 to 2020, prices were still increasing, but at a rather moderate average growth rate of 2.5% a^{-1}. Looking at these developments in the context of monetary dynamics, electricity prices have hardly increased at all in recent years. Whereas the inflation rate between 2013 and 2019 averaged 0.98% a^{-1}, the electricity price grew by only 0.82% a^{-1} in the same period. Thus, compared to the average consumer price basket, the electricity price increased below-average during that time and shows a slightly decreasing chart between 2013 to 2020 in real terms, followed by a slight increase in the first half of 2021 (cf. Figure 4). This indicates a rather emotionally driven debate on the development of electricity prices instead of an objective discussion during that period.



(**a**) (**b**)

Figure 3. Development of nominal end customer prices: (**a**) Nominal price developments of electricity and natural gas for private households in Germany from 1950 until the second quarter of 2021 (natural gas from 1970 due to lack of data for previous decades). Data based on [47–50]. (**b**) Nominal price developments of petrol for private customers in Germany from 1950 to 2020. Data based on [47].



(**a**) (**b**)

Figure 4. Nominal and real electricity prices for private end consumers and development of average gross incomes: (**a**) Development of nominal and real German end consumer electricity prices until the end of the second quarter 2021. Calculation of real prices in Euro$_{2020}$ according to the consumer price index [47,49,50]. (**b**) Comparison of the average gross income to nominal and real (Euro$_{2020}$) electricity prices in percent and normalized to 1975 = 100% [51].

Looking at the electricity price trends further back, it can be seen that the price level of 2020 in real Euro_{2020} is well below that of the 1950s (Figure 4a). Figure 4b shows the development in comparison to the average gross income of German employees. Normalized to 1975, the average gross income increased by 450%, whereas electricity in Euro_{2020} increased by 150%. However, the electricity price can still be considered critical for households with low incomes because the growth rate of the average gross income is mainly driven by the fraction with very high incomes. Thus, despite the moderate real term price development, political action is required if low-income households are overburdened by electricity prices. The current situation, with both comparably high costs for electricity as well as for heating and mobility, displays the requirement for a financial relief. Nevertheless, it is noteworthy that the recent price dynamics are correlated to fossil energy carriers only, whereas energy from renewable sources is available at stable prices.

Historic price developments of natural gas for private households as well as for industry customers have revealed strong fluctuations since 1970 according to Figures 3a and 5 as they are correlated to the fluctuating crude oil price trends. From 1971 to 1980, industry prices grew by an extraordinary 27.5% a^{-1} on average as a result of the oil price crisis, followed by a slight average decline of −0.27% a^{-1} from 1981 to 1990. In the 2000s, a high averaged growth rate of 4.7% a^{-1} from 2001 to 2010 was followed by an average decline of −3.6% a^{-1} from 2011 to 2020.

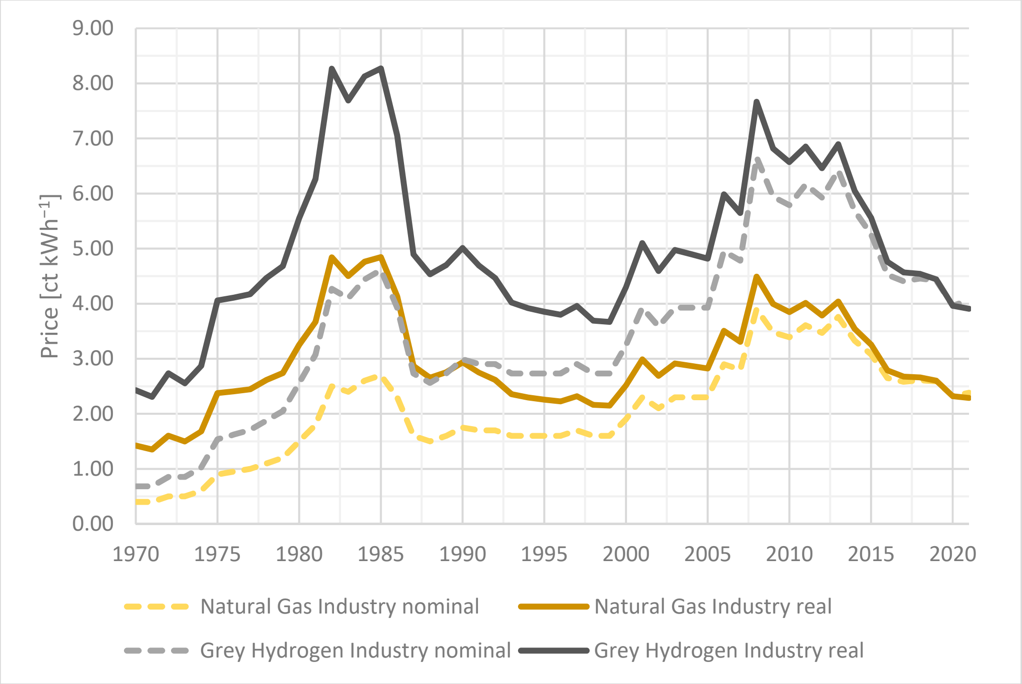


Figure 5. Development of nominal and real (ct_{2020}) natural gas and grey hydrogen prices for industry customers from 1970 to 2020 [48,49]. Prices for grey hydrogen are based on own calculations.

Due to the correlation with the natural gas price, production costs of grey hydrogen followed a comparable pattern. With expected natural gas prices of up to 5 ct kWh^{-1} in 2050, the production costs of grey hydrogen will reach a price level >8 ct kWh^{-1}, which is comparable to its real production costs in the early 1980s. Grey hydrogen prices in March 2022 instead rose to an extraordinary 32.2 ct kWh^{-1} and thus clearly exceed the above stated green hydrogen production cost ranges via water electrolysis.

Nevertheless, the projected future natural gas prices come with average growth rates from 2.5–3.3% a^{-1} until 2050 (cf. Section 2.1). These are higher than the targeted inflation rate of 2% a^{-1} according to the fiscal policy strategy of the European Central Bank (ECB), but lower than the average price growth rates of the 1970s and 2000s [52]. Thus, even though the expected price developments can be considered moderate compared to earlier decades, the steadily increasing price trend urges a switch to renewable energy sources such as green hydrogen.

Regarding the development of crude oil products such as petrol since 1970, strong price fluctuations in both directions appeared occasionally, but followed an overall increasing trend. Price peaks were usually caused by international crises. While the average petrol customer price in the year 2000 was around 101 ct l^{-1}, it reached an all-time high in 2012 with 165 ct l^{-1} and declined again to 129 ct l^{-1} in 2020 (all including taxes) (cf. Figure 3b). In real terms, petrol prices peaked during the period 2011–2013 with 171–180 ct_{2020}/l^{-1} (including taxes). Crude oil reached an all-time high in 2012 with 6.7 ct kWh^{-1} (7.3 ct_{2020} kWh^{-1}) and fell to 2.55 ct kWh^{-1} in 2020, followed by a new all-time high in 2022 with 8.7 ct kWh^{-1}. Price projections until 2050 show a maximum price of <7 ct kWh^{-1}, meaning nearly a triplication compared to 2020, but hardly any difference compared to 2012.

Looking at the expected price developments for green hydrogen and synthetic fuels, it was revealed in Section 2.1 that green hydrogen will reach comparable production costs to former natural gas prices by 2050. The defined benchmark prices in Section 2.2 for natural gas could be undercut by green hydrogen by the end of the 2020s, and those for crude oil products and grey hydrogen in the best-case assumptions already in 2020. Synthetic fuels remain clearly more expensive than crude oil price projections until 2050 but could reach production costs that are comparable to crude oil price peaks in 2022 and to consumer prices of petrol in 2020.

Actual prices for natural gas and crude oil-based products of late 2021 and early 2022 clearly overshoot short-term green hydrogen production costs. Hence, socio-economic disruptions are currently caused by the conventional energy supply system, with heavy consequences for the overall (global) economy. Commerce and industries as well as private households are confronted with partially unaffordable energy prices, leading to self-reinforcing effects for global supply chains, a decline in purchasing power, and consequentially to high inflation rates [53]. Instead, a gradual implementation of the renewable substitutes is unlikely to cause such sudden price surges and economic constraints; as for the application of green hydrogen, a gradual incorporation into industrial processes is planned to stepwise substitute grey hydrogen and hydrocarbon-based fuels. In the mobility sector, hydrogen fueling stations usually deliver a mix with increasing shares of green hydrogen. Synthetic fuels can be implemented as drop-in fuels, e.g., in the aviation sector, with increasing shares over time. Thus, even under the assumption of decreasing energy prices back to early 2021 levels, the (intermediate) higher expenses for the renewable substitutes should not cause heavy price surges for customers. In addition, to support both a straightforward implementation of renewable energies in all sectors as well as moderate energy prices, strong financial incentives via subsidization mechanisms should be applied anyway.

4. Conclusions

It was shown that, contrary to what is often portrayed in energy price debates, there have hardly been any drastic price increases for electricity, natural gas, or crude oil-based fuels in recent years prior to the energy crisis beginning in the second half of 2021. Moreover, all discussed products were significantly more expensive in earlier periods. Especially under consideration of the developments of gross incomes and the consumer price index, there can be no evidence-based talk of an excessive financial burden from energy prices for the average customer until the first half of 2021.

Instead of energy being too expensive, in a holistic view the problem is the generally too-low overall energy price level in comparison to the determined benchmark prices, entailing high downstream costs in the long-term. In addition, the recent extremely high energy price levels show that the fossil-based energy supply is rather fragile in times of geopolitical crises and can cause recessions for whole economies as a consequence of sudden unpredictable price surges. The implementation of renewable substitutes such as green hydrogen and synthetic fuels alongside expanding efficiency measures and an increased direct electrification, as well as high renewable power generation capacities, can enable both lower long-term downstream costs as well as better price stabilities.

In Schnuelle et al., it was stated that a large-scale implementation of green hydrogen and synthetic fuels in Germany may cause additional national energy costs of 10–100 billion Euro a^{-1} compared to an ongoing fossil fuel supply at constant price conditions at 2020 price levels [54]. However, by applying the above-discussed environmental impact costs to the overall German greenhouse gas emissions of 2019, a hypothetic bill as high as 156 billion Euro arises and thus causes considerably higher annual expenses for the German economy.

The calculated benchmark prices are well above historic price peaks, but lower than the recent price peaks in the first quarter of 2022, which caused high financial burdens for private and commercial customers. Because the renewable substitutes also come at comparably high prices in the short-term, policy makers need to consider how to financially relieve customers and concurrently promote a rapid implementation. In this context, policy measures should focus on the promotion of energy savings in the form of sufficiency and efficiency measures as well as an adaption to more climate-friendly behavior patterns, e.g., motivation to use public transport instead of own cars. This could be realized via a carbon tax system, as already implemented in Canada and Switzerland, and proposed by Bach et al., which provide an indirect fixed refund per capita in the form of a 'climate bonus' [55]. Typical further instruments can be financial compensations at least for low incomes or prohibitive tariffs for commodities that are produced in a fossil energy-based supply chain. In the medium and long-term, such efforts will pay off as green hydrogen is expected to become the cheapest fuel of those considered in this study over time, with a steep cost degression of approximately 32% from 2022 till 2030.

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Appendix

Accompanying Research Papers of the Dissertation Project

A: Multikriterielle Bewertung von Elektrolyse- und CO_2-Capture Technologien für eine Power-to-Methanol Prozesskette

B: Ausgewählte Standortfaktoren für Power-to-Fuel Anlagen: Erdölraffinerie versus grüne Wiese

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Multikriterielle Bewertung von Elektrolyse und CO_2-Capture Technologien für eine Power-to-Methanol Prozesskette

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Diesen Artikel widmen wir unserem ehemaligen Arbeitsgruppenleiter und Mentor Prof. Dr. Stefan Gößling-Reisemann, der uns inspiriert, sein Wissen mit uns geteilt und sich mit großer Leidenschaft für die Energieforschung sowie eine nachhaltige Zukunft eingesetzt hat.

Abstract

Im Kontext der Energiewende und aktuellen Anstrengungen zur Reduktion von Treibhausgasemissionen erfahren Power-to-X Prozesse zunehmend Beachtung, da Sie die Minderung von Emissionen in schwer zu defossilisierenden Sektoren wie der chemischen Industrie oder dem Flugverkehr ermöglichen. Die Auswahl geeigneter Technologiealternativen für die Prozessstufen der Wasserstofferzeugung und der CO_2-Abscheidung stellt unter Berücksichtigung multipler Kriterien eine Herausforderung in der Gestaltung solcher Power-to-X Prozesse dar. Im Rahmen dieser Arbeit wird eine multikriterielle Bewertung im Rahmen einer Fallstudie für verschiedene Elektrolyse und CO_2-Capture Technologien auf Basis ökonomischer, ökologischer und technischer Kriterien vorgenommen. Die ausgewählte Fallstudie betrachtet den Anwendungsfall einer Power-to-Methanol Prozesskette am Standort der Raffinerie Heide in Schleswig-Holstein. Die Analyse und Bewertung werden auf Basis der etablierten Methoden des Analytical Hierarchy Process und der Nutzwertanalyse durchgeführt. Für den Prozessschritt der Wasserstofferzeugung wurden die alkalische und die Protonen-Austausch-Membran-Elektrolyse jeweils in einer Hoch- und einer Niederdruck Ausführung berücksichtigt. Für die CO_2-Abscheidung wurde zwischen einem Niedertemperatur Direct Air Capture Verfahren und einer Abscheidung aus dem raffinerieeigenen Kraftwerksrauchgasstrom mittels Aminwäsche differenziert. Die Analyse zeigt, dass eine atmosphärisch betriebene alkalische Elektrolyse, unter Berücksichtigung von insgesamt 10 Kriterien, die präferierte Technologie zur Wasserstoffbereitstellung darstellt. Kohlenstoffdioxid sollte entsprechend der ausgeführten Bewertung unter Berücksichtigung von 6 Kriterien vorzugsweise durch Aminwäsche aus den raffinerieeigenen Kraftwerksrauchgasen abgeschieden werden.

Keywords: MCDA, Power-to-X, multikriterielle Bewertung, Elektrolyse, CO_2-Abscheidung

Abkürzungen

AEL	Alkalische Elektrolyse
AHP	Analytical Hierarchy Process
CAPEX	Capital expenditure
DAC	Direct Air Capture
HP	High Pressure
HT	High temperature
KWK	Kraft-Wärme-Kopplung
LP	Low Pressure
LT	Low temperature
MADM	Multi-Attribute Decision Making
MCDA	Multi Criteria Decision Analysis
MODM	Multi-Objective Decision Making
OPEX	Operational expenditure
MeOH	Methanol
PEMEL	Protonen-Austausch-Membran-Elektrolyse
PtX	Power-to-X
TRL	Technology Readiness Level

1. Einleitung

Ein weltweit kontinuierlich steigender Energiebedarf, damit einhergehend ebenfalls zunehmende klimawirksame Emissionen sowie die Ausbeutung fossiler Ressourcen erfordern eine drastische und zeitnahe Transformation der Energie- und Rohstoffversorgung. Durch den Ausbau von erneuerbaren Energien, insbesondere in Form von Photovoltaik und Windenergieanlagen, konnte im Jahr 2019 bereits ein Anteil von 46,1 % der deutschen Stromerzeugung regenerativ bereitgestellt werden [1]. Für den Ausgleich der volatilen Erzeugung und eine Integration des erneuerbaren Stroms in andere energieintensive Sektoren bedarf es allerdings zunehmend neuer Speichertechnologien und Konversionsverfahren. Insbesondere die Erzeugung strombasierter, synthetischer Basischemikalien und Kraftstoffe durch so genannte Power-to-X Konzepte stellt einen vielversprechenden Ansatz zur Reduzierung von Treibhausgasemissionen in nur schwer zu defossilisierenden Anwendungen und zur Kopplung der Sektoren Strom, Industrie und Verkehr dar [2].

Durch die Herstellung von Elektrolyse-Wasserstoff können bisher abgeregelte Erzeugungsspitzen geglättet und chemisch gespeichert werden. Mit einer nachhaltigen CO_2-Quelle können in einem Synthese-Schritt langkettige Kohlenwasserstoffe synthetisiert werden, welche beispielsweise als Drop-In Kraftstoffe in bereits vorhandene Infrastrukturen integriert und in andere Sektoren ausgekoppelt werden können. Die entsprechenden Technologien solcher Prozessketten sind bereits auf unterschiedlichen Skalen entwickelt, leiden allerdings unter hohen Investitions- und Betriebskosten sowie an zum Teil noch geringer Effizienz und Flexibilität. Für die Realisierung großer PtX Anlagen stellt sich daher je nach den standortspezifischen Rahmenbedingungen die Frage nach einer optimalen Technologieauswahl für die Ausgestaltung der Prozesskette. Unter Berücksichtigung technischer, wirtschaftlicher und ökologischer Kriterien bietet sich für die Identifizierung einer am besten geeignetsten Prozesskette die Durchführung einer multikriteriellen Bewertung an. Mittels etablierter Methoden, wie dem Analytical Hierarchy Process (AHP) und der Nutzwertanalyse, wird im Rahmen dieser Ausarbeitung eine Technologieempfehlung für eine Power-to-Methanol Anlage am Standort der Raffinerie Heide in Schleswig-Holstein erarbeitet. Konkret werden die Prozessschritte Elektrolyse und Carbon Capture betrachtet, die im Kontext einer strombasierten Kohlenwasserstoffsynthese zur H_2/CO_2 Versorgung dienen. In den folgenden Abschnitten werden zunächst die standortspezifischen Rahmenbedingungen dargestellt (Abschnitt 2) und das methodische Vorgehen der multikriteriellen Bewertung skizziert (Abschnitt 3). In Abschnitt 4 werden die Ergebnisse dargestellt und diskutiert und abschließend in Abschnitt 5 zusammengefasst.

2. Fallstudie Power-to-Methanol am Standort Raffinerie Heide

Für eine großskalige Umsetzung von PtX Anlagen bieten industrielle Bestandsprozesse, für deren Betreiber die Herstellung strombasierter Produkte einen ökonomischen und/oder ökologischen Mehrwert darstellt, aus heutiger Sicht ideale Einstiegsbedingungen. Erdölraffinerien, wie die Raffinerie Heide, weisen ein besonders attraktives Umfeld auf, da Erfahrung in der Verarbeitung von Kohlenwasserstoffen vorliegt, notwendige Infrastrukturen vorhanden sind, bestehende CO_2-Rauchgasströme als Punktquellen zur Verfügung stehen und im Rahmen umweltregulatorischer Verpflichtungen neue Lösungen für das Inverkehrbringen klimafreundlicherer Kraftstoffe gesucht werden [3]. Darüber hinaus bietet sich das Bundesland Schleswig-Holstein mit seiner hohen Kapazität an Onshore- und Offshore-Windenergieanlagen und weiteren hohen Ausbaupotentialen als Modellregion für großskalige PtX Projekte an [4]. Derzeit sind in Schleswig-Holstein Onshore-Windenergieanlagen mit einer Nennleistung von 6,7 GW installiert [5]. Im Zusammenspiel mit einem unzureichenden Netzausbau führte dies auf Bundeslandebene zu Ausfallarbeit in Höhe von 3.258 GWh in 2017 und 2.860 GWh in 2018 [5], [6].

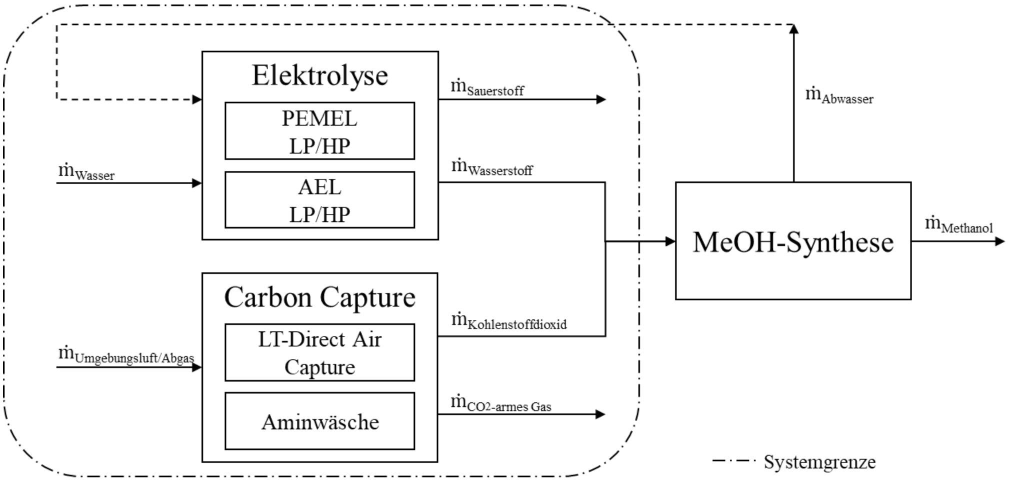

Abbildung 1: Prozessschema inkl. berücksichtigter Technologien und Systemgrenze

Für die Fallstudie „Power-to-Methanol am Standort Raffinerie Heide“ wird eine elektrische Anlagennennleistung in Höhe von 200 MW definiert, die einer industriellen Anlage mit einem Methanoloutput von circa 152 kt/a entspricht [3]. Wie in Abbildung 1 dargestellt, werden verschiedene Technologieoptionen für die Prozessschritte Elektrolyse und Carbon Capture im Gesamtkontext einer Power-to-Methanol Anlage betrachtet. Für die Wasserstoffbereitstellung werden die alkalische Elektrolyse (AEL) und die Protonen-Austausch-Membran-Elektrolyse (PEMEL) jeweils für den Betrieb bei atmosphärischem Druck (LP) und bei 30 bar (HP) berücksichtigt. Um die Vergleichbarkeit beider Druckniveaus im Kontext des spezifischen Anwendungsfalls zu gewährleisten, wird jeweils eine

Nachverdichtung auf 75 bar berücksichtigt. Dies stellt ein typisches Druckniveau für die Methanolsynthese über direkte Hydrierung dar [7]. Eine Besonderheit der PEMEL, die im Rahmen der weiteren Analyse aufgegriffen wird, ist ihre Fähigkeit Wasser zu verarbeiten, das eine Methanolbelastung aufweist. Tatsächlich wurde für die PEMEL ein erhöhter Wirkungsgrad bei Verwendung von MeOH-belasteten Wasser beschrieben [8]. Diese Fähigkeit grenzt PEMEL und AEL im Analysefall Power-to-Methanol voneinander ab, da die AEL mit hochreinem, deionisiertem Wasser zu versorgen ist.

Als potentielle CO_2-Quellen werden im Rahmen dieser Arbeit die Umgebungsluft sowie das KWK-Kraftwerk der Raffinerie Heide betrachtet. Die CO_2-Abscheidung aus Umgebungsluft wird in Form des Direct Air Capture Verfahrens von Climeworks berücksichtigt, das eine Regeneration des Sorbents bei einem niedrigen Temperaturniveau (LT) von 100° C ermöglicht [9]. Aufgrund der niedrigen CO_2 Konzentration von 0,0407 vol.-% in der Umgebungsluft, ist die Abscheidung im Vergleich zu konzentrierten Punktquellen thermodynamisch aufwändiger. Die Abscheidung aus dem KWK-Kraftwerk der Raffinerie Heide wird über die etablierte Technologie Aminwäsche, unter Anwendung von Monoethanolamin (MEA) als Waschmittel, berücksichtigt. Das Kraftwerk stellt bezogen auf die emittierte CO_2 Menge mit circa 50 t_{CO2}/h die größte CO_2-Punktquelle am Standort dar und weist eine CO_2 Konzentration in Höhe von etwa 10 vol.-% auf.

3. Methodisches Vorgehen bei der Multi Criteria Decision Analysis (MCDA)

Mit MCDA Methoden können Ergebnisse für ein Entscheidungsproblem erzielt werden, die eine Vielzahl an (interdisziplinären) Kriterien berücksichtigen und somit als eine Grundlage oder Handlungsempfehlung für wichtige Entscheidungen dienen können. Innerhalb etablierter Methoden zur multikriteriellen Analyse von Entscheidungsproblemen wird zwischen den Bereichen des „Multi-Objective Decision Making“ (MODM) und des „Multi-Attribute Decision Making“ (MADM) differenziert. Bei MODM Methoden werden optimale Lösungen aus einer stetigen Menge an Alternativen mittels mathematischer Verfahren ermittelt. Dem gegenüber werden bei MADM Methoden verschiedene diskrete Alternativen in Hinblick auf spezifische Kriterien bewertet [10]. Im Vorfeld der Entscheidungsfindung liegen also die zu betrachtenden Alternativen exakt definiert vor und das Entscheidungsproblem wird nach einer bestmöglichen Auswahl gelöst. Übertragen auf den konkreten Anwendungsfall für den Standort Raffinerie Heide kann also auf Basis der Charakterisierung von Einzeltechnologien mit MADM Methoden die Frage nach den am besten geeignetsten Technologien für eine Power-to-Methanol Anlage beantwortet und eine Technologieempfehlung gegeben werden.

Methodisch werden für die MCDA in dieser Ausarbeitung die klassischen Verfahren der Nutzwertanalyse und des Analytical Hierarchy Process (AHP) angewendet, welche den Präferenzen des Entscheidungsträgers eine Nutzfunktion bzw. einen Nutzenwert zuordnen.

3.1 Schrittabfolge einer MCDA

Die Durchführung einer MCDA durchläuft in der Regel folgende Schrittabfolge, wobei die einzelnen Schritte nicht exakt definiert sind und zum Teil nochmals in weitere Einzelschritte unterteilt werden (vgl. [11], [12]).

1. Entscheidungsproblem definieren
2. Identifikation der Alternativen

3. Beschreibung des Zielsystems
4. Bestimmung der Kriterien und Darstellung in einer Hierarchie
5. Definition der Kriterienausprägungen für die einzelnen Alternativen
6. Ermittlung der subjektiven Kriteriengewichtung
7. Aggregation und Erzielen einer Rangfolge

Zunächst wird für die Durchführung einer MCDA ein Entscheidungsproblem definiert. Da das Entscheidungsproblem zumeist mehrere Faktoren umfasst, sollte an dieser Stelle ein übergeordnetes Gesamtziel formuliert werden, welches das Problem vollständig erfasst. Im zweiten Schritt werden bei MADM Methoden diskrete Alternativen definiert und beschrieben. Alternativen bilden die Wahlmöglichkeiten für die Lösung des Entscheidungsproblems, folglich müssen mindestens zwei Alternativen vorliegen. Für eine Vergleichbarkeit müssen diese mit charakteristischen Merkmalen beschrieben bzw. mit Daten unterlegt werden, wobei die Daten für alle Alternativen gleichermaßen vorliegen müssen.

Häufig wird bei der Entscheidungsfindung mehr als ein Ziel verfolgt und zwischen den parallel verfolgten Zielen bestehen zumeist Abhängigkeiten. Darüber hinaus können die Ziele auch in Widerspruch zueinander stehen. Im dritten Schritt gilt es daher ein strukturiertes Zielsystem zu definieren, für welches zunächst ein das Gesamtziel widerspiegelndes, jedoch meist abstrakteres, Oberziel formuliert wird. Im Anschluss werden spezifischere Unterziele definiert, mittels derer die exakten Ziele konkretisiert werden. Das Zielsystem stellt damit auch die Grundlage für die Ermittlung einer Kriterienhierarchie dar.

Die relevanten Kriterien können im vierten Schritt auf Basis des Zielsystems definiert werden. Sie stellen eine Grundlage zur Operationalisierung von (Unter-)Zielen dar und müssen in einem logischen Zusammenhang mit einem der (Unter-)Ziele stehen. Um die Zusammenhänge zu verdeutlichen, bietet es sich an, eine Kriterienhierarchie zu erstellen, durch welche das Entscheidungsproblem von Ebene zu Ebene immer detaillierter dargestellt wird. Dafür werden auf höchster Ebene grob definierte Oberziele aufgeführt, die anschließend über die Zuordnung von Unterzielen aufgeschlüsselt werden. Für die Unterziele werden dann passende Kriterien aufgeführt, welche abschließend in Form von messbaren Attributen konkretisiert werden. Den Attributen werden eine Maßeinheit und das Ziel einer Maximierung oder Minimierung zugeordnet.

Im fünften Schritt werden den Kriterien konkrete Werte, so genannte Kriterienausprägungen, zugeteilt, welche auf Basis einer Literaturrecherche und Expertenbefragungen erhoben werden. Der Entscheidungsträger kann seine (subjektive) Einschätzung einfließen lassen, wie wichtig die einzelnen Kriterien hinsichtlich des Gesamtproblems sind. Die Gewichtung bzw. der Gewichtungsfaktor repräsentiert also die Bedeutsamkeit des Kriteriums und stellt den sechsten Schritt in der Durchführung einer MCDA dar. Die Ermittlung der Gewichtungsfaktoren stellt eine Herausforderung dar, da sie im Prinzip immer auf der subjektiven Einschätzung des Entscheiders beruht. Häufig werden Gewichtungsfaktoren auf einem kardinalen Skalenniveau dargestellt, welches üblicherweise von 0-100 Punkten oder 0-100 % reicht. Es gibt zahlreiche Methoden, die zur Ermittlung einer Kriteriengewichtung zum Einsatz kommen. Weit verbreitet ist der von Thomas L. Saaty entwickelte Analytical Hierarchy Process (AHP), welcher in dieser Ausarbeitung genutzt und nachfolgend zusammenfassend erläutert wird [13].

Beim AHP werden Wertefunktionen gebildet, deren Werte durch Paarvergleiche, also dem jeweiligen Vergleich zweier Elemente gegenüber einem anderen Element, von Kriterien ermittelt werden. Mithilfe der so genannten Saaty-Skala werden jeweils zwei Elemente paarweise bezüglich ihrer relativen Wichtigkeit zu einem weiteren Element verglichen. Die Saaty-Skala besteht aus einem 9-Punkte Bewertungssystem, welches in Tabelle 1 dargestellt wird. Den Kriterien werden gemäß der Skala je nach ihrer Bedeutung gegenüber des zu vergleichenden Kriteriums die Punkte 1-9 vergeben. Wird einem Kriterium die gleiche Bedeutung bzw. Wichtigkeit gegenüber dem Vergleichskriterium zugeordnet, so wird es mit 1 bewertet. Wird ein Kriterium als dominierend eingestuft, erhält es höhere Werte bis maximal 9 Punkte [14].

Tabelle 1: Saaty-Skala zur Bewertung von Kriterien

Skalenwert	**Bedeutung**
1	Gleiche Bedeutung
3	Etwas größere Bedeutung
7	Deutlich größere Bedeutung
9	Absolut Dominierend
2, 4, 6, 8	Zwischenwerte

Die Saaty-Skala kann sowohl für quantifizierbare als auch qualitativ beschriebene Kriterien genutzt werden. Für jedes Kriterium *C* wird eine $n \times n$ Matrix *A* aufgestellt, deren Komponenten a_{ij} ($i, j = 1, 2, ..., n$) numerische Einträge darstellen, welche die relative Bedeutung des Kriterium *i* gegenüber Kriterium *j* ausdrücken [15].

Nach Durchführung der paarweisen Vergleiche ergibt sich eine Matrix *A* der Form:

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} \qquad 1$$

mit $a_{ii} = 1$, $a_{ji} = a_{ij}$ und $a_{ij} \neq 0$.

Die Zielgewichte können anschließend mittels verschiedener Verfahren bestimmt werden. Zwei gängige Ansätze sind die Bestimmung des geometrischen Mittels oder des Eigenvektors der Matrix *A* zum größten Eigenwert. Die von Saaty vorgeschlagene Methode ist hierbei die Bestimmung des Eigenvektors, da dieser auch für eine folgende Konsistenzüberprüfung verwendet werden kann [16]. Der Eigenvektor $\vec{v}$ ist dabei eine nicht-triviale Lösung (kein Null-Vektor) welcher der Gleichung 1 genügt. Hier repräsentieren λ_{max} den maximalen Eigenwert und E die Einheitsmatrix.

$$(A - \lambda_{max} \cdot E) \cdot \vec{v} = 0 \qquad 2$$

Zur Bestimmung des maximalen Eigenwerts wird das charakteristische Polynom mithilfe der in Gleichung 3 und 4 gezeigten Determinanten gebildet und gelöst.

$$\det(A - \lambda_{max} \cdot E) = 0 \qquad 3$$

$$det \begin{pmatrix} a_{11} - \lambda_{max} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} - \lambda'\lambda_{max} & \dots & a_{2n} \\ \dots & \dots & \ddots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} - \lambda_{max} \end{pmatrix} = 0 \qquad 4$$

Der größere Aufwand der Eigenwert-Methodik im Vergleich zur Berechnung des geometrischen Mittels ermöglicht eine nachfolgende Konsistenzüberprüfung der paarweisen Vergleiche der Kriterienbedeutungen. Der zuvor berechnete maximale Eigenwert λ_{max} kann dafür nach Gleichung 5 in einen Konsistenzindex (*CI*) überführt werden und mit einem Zufallsindex (*RI*) nach Gleichung 6 zum Konsistenzverhältnis (*CR*) ins Verhältnis gesetzt werden. Wenn das gebildete Verhältnis *CR* < 0,1 ist, entspricht dies einer genügend konsistenten Vergleichsmatrix.

$$CI = \frac{\lambda_{max} - n}{n - 1} \qquad 5$$

$$CR = {}^{CI}/_{RI} \qquad 6$$

Eine Übersicht über die von Saaty berechneten Zufallsindizes *RI* gibt Tabelle 2.

Tabelle 2: Zufallsindizes RI in Abhängigkeit der Kriterienanzahl n [16]

n	3	4	5	6	7	8	9	10
RI	0,58	0,9	1,12	1,24	1,32	1,41	1,45	1,49

Nach Prüfung der ausreichenden Konsistenz der paarweisen Kriterienvergleiche, wird im letzten Schritt eine Methode zur Aggregation der zuvor durchgeführten Arbeiten ausgewählt. In dieser Ausarbeitung wird die Nutzwertanalyse angewendet (vgl. [17], [18]). Um die multiattributive Bewertung einer Alternative in einen eindimensionalen Nutzwert transponieren zu können, müssen die Kriterienausprägungen miteinander vergleichbar gemacht werden. Eine Berücksichtigung aller Kriterien kardinal in ihrer jeweiligen Dimension würde zu stark abweichenden Werten in den Spalten-Vektoren führen. Ohne Normalisierung würden dadurch implizite Gewichtungen der Kriterien aufgrund von Skaleneffekten entstehen. Aus diesem Grunde wird hier in Abhängigkeit der Wirkrichtung des Kriteriums eine lineare Normalisierung vorgenommen und ein dimensionsloser Parameter berechnet. Je nach Wirkrichtung wird beim Ziel einer Minimierung der niedrigste Wert eines Kriteriums auf 1 normalisiert, beim Ziel einer Maximierung wird der höchste Wert gleich 1 gesetzt.

In einem nächsten Schritt werden aus den Gewichtungen und normalisierten Parametern Nutzwerte berechnet, wobei jeweils das Produkt aus den Gewichten der Kriterien und den Parametern gebildet wird. Aus der Summe der so berechneten Nutzwerte ergibt sich der Gesamtnutzwert einer Alternative und es kann abschließend eine Rangfolge gebildet werden.

$$Gesamtnutzwert\ (A_1) = \sum_{r=1}^{n} Gewichtung_r \times normalisierter\ Parameter_r \qquad 7$$

3.2 Anwendung der Methoden

Bezogen auf die übergeordnete Fragestellung, der Bestimmung einer für den Standort optimalen Technologieauswahl für die Prozessschritte Elektrolyse und CO_2-Capture, wird das Entscheidungsproblem für die beiden Technologien separat behandelt. Für den Prozessschritt Elektrolyse werden die vier Alternativen AEL (LP), AEL (HP), PEMEL (LP) und PEMEL (HP) bewertet. Das Hochtemperaturverfahren Festoxid-Elektrolyse wird aufgrund des noch vergleichsweise geringen Technology Readiness Level (TRL) von 5-6 nicht mit in die Bewertung mit aufgenommen.

Für die Analyse werden technische, wirtschaftliche und ökologische Aspekte betrachtet. Das Zielsystem setzt sich somit aus den Unterzielen einer technischen Funktionalität/Plausibilität, wirtschaftlicher

Effizienz und geringer ökologischer Wirkungen zusammen. Für eine exakte Beschreibung der Unterziele wird gemäß Abbildung 2 eine Kriterienhierarchie gebildet, für die geeignete Kriterien unter Berücksichtigung der jeweiligen Wirkrichtung (Maximierung vs. Minimierung) definiert werden. Insgesamt wurden zehn Kriterien zur Lösung des Entscheidungsproblems bestimmt, von denen fünf der technischen Funktionalität, zwei der Wirtschaftlichkeit und drei den ökologischen Wirkungen zugeordnet werden. Die für jedes Kriterium erhobenen Daten sind in Tabelle 3 und Tabelle 4 dargestellt.

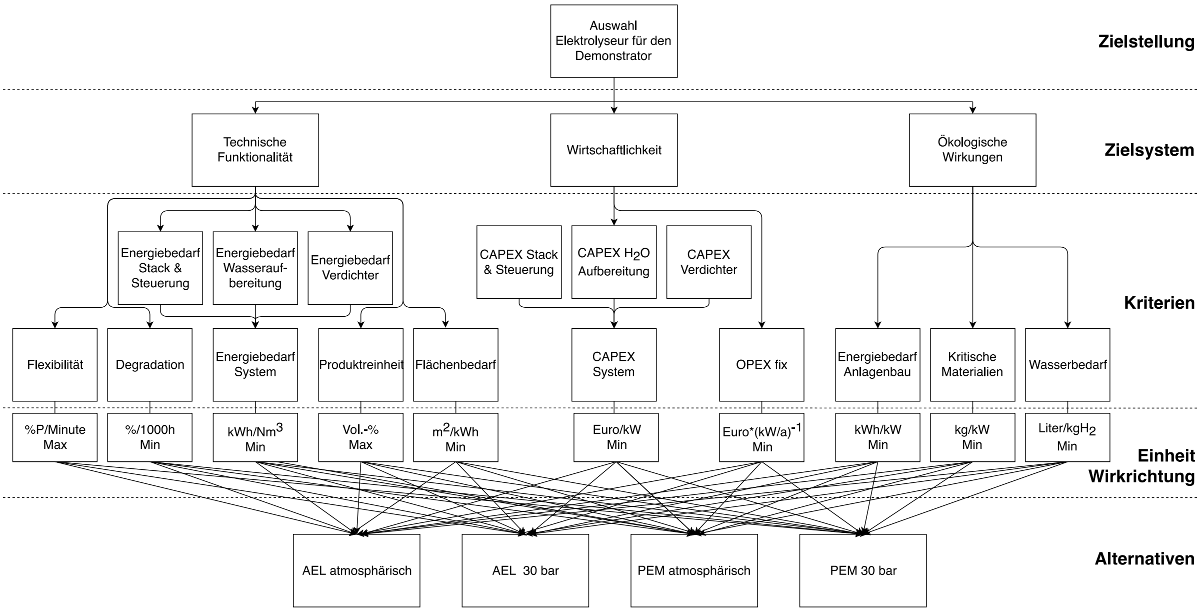

Abbildung 2: Darstellung der Kriterienhierarchie für die Auswahl eines am besten geeigneten Elektrolyseurs.

Aufgrund der Gegenüberstellung von Druck- und atmosphärischer Elektrolyse sowie der Option einer Abwasserrückführung aus der Methanolsynthese sind die Kriterien Energiebedarf und CAPEX zur weiteren Spezifizierung entsprechend in drei Unterkriterien unterteilt und werden jeweils zu einem Gesamtwert für das Elektrolyse-System aggregiert. Unter den fixen OPEX werden Kosten für die Wartung der Anlage aufgeführt. Variable Kosten für die Betriebsmittel Strom und Wasser werden nicht gesondert als Kriterium mit aufgenommen, da sie bereits indirekt über die Kriterien Energie- und Wasserbedarf abgedeckt sind und zu einer impliziten Verschiebung der Gewichtungen führen würden. Die Werte zu kritischen Materialien beziehen sich auf den Einsatz von Platingruppenmetallen, welche nur bei PEM-Elektrolyseuren eingesetzt werden (vgl. [2]).

Die MCDA wird für den Prozessschritt Elektrolyse für zwei Betrachtungsfälle durchgeführt. Wie in Abschnitt 2 bereits einführend erläutert, wird in der Literatur die Option der Verarbeitung von Wasser mit Methanolbelastung bei der PEM-Elektrolyse diskutiert. Diese Option würde die Rückführung des Abwasserstroms zur PEM-Elektrolyse ermöglichen und den Gesamtprozess effizienter gestalten, da sich einerseits der Wasserbedarf der gesamten Prozesskette und andererseits der Anteil des aufzubereitenden Speisewassers für die Elektrolyse entsprechend reduzieren ließen. Bisher ist die Umsetzung einer solchen Betriebsführung allerdings nicht bekannt, so dass hier in den Betrachtungsfällen bezüglich der Möglichkeit einer Abwasserrückführung differenziert wird. Die Parameter für alle Kriterien im Betrachtungsfall 1 ohne die Option einer Abwasserrückführung sind in Tabelle 3 dargestellt, für Betrachtungsfall 2 in Tabelle 4.

Tabelle 3: Übersicht über die Parametrierung der berücksichtigten Kriterien für Betrachtungsfall 1 – Keine Abwasserrückführung aus der MeOH-Synthese zur PEM-Elektrolyse [19][20][21][22][23][24][25][26][27][28][29].

Kriterium / Alternative	**Einheit**	**Min/Max**	**AEL LP**	**AEL HP**	**PEMEL LP**	**PEMEL HP**
Energiebedarf Elektrolyse	kWh/Nm^3	Min	4,5	5,4	4,7	4,8
Energiebedarf H_2O Aufbereitung	kWh/Nm^3	Min	0,18	0,18	0,18	0,18
Energiebedarf Verdichtung	kWh/Nm^3	Min	0,25	0,05	0,25	0,05
Energiebedarf System	kWh/Nm^3	Min	4,93	5,63	5,13	5,03
Flexibilität	%P/min	Max	20	20	100	100
Degradation	$\%_{\eta}$/1000h	Min	0,13	0,13	0,2	0,2
Produktreinheit	Vol.-%	Max	99,9	99,9	99,99	99,99
Flächenbedarf	m^2/MW	Min	63	63	14,48	14,48
CAPEX Elektrolyse	€/kW	Min	709	850	1363	1450
CAPEX H_2O Aufbereitung	€/kW	Min	6	6	6	6
CAPEX Verdichtung	€/kW	Min	62	9,1	62	9,1
CAPEX System	€/kW	Min	777	866	1431	1465
OPEX fix	€·(kW/a)$^{-1}$	Min	15,08	23,08	12,04	15,04
Energiebedarf Anlagenbau	kWh/kW	Min	5,74	5,74	7	7
Kritisches Material	kg/kW	Min	0	0	0,0006	0,0006
Wasserbedarf	l/kg	Min	15	15	15	15

Tabelle 4: Übersicht über die Parametrierung der berücksichtigten Kriterien für Betrachtungsfall 2 – Abwasserrückführung aus der MeOH-Synthese zur PEM-Elektrolyse [19][20][21][22][23][24][25][26][27][28][29].

Kriterium / Alternative	**Einheit**	**Min/Max**	**AEL LP**	**AEL HP**	**PEMEL LP**	**PEMEL HP**
Energiebedarf Elektrolyse	kWh/Nm^3	Min	4,5	5,4	4,7	4,8
Energiebedarf H_2O Aufbereitung	kWh/Nm^3	Min	0,18	0,18	0,13	0,13
Energiebedarf Verdichtung	kWh/Nm^3	Min	0,25	0,05	0,25	0,05
Energiebedarf System	kWh/Nm^3	Min	4,93	5,63	5,08	4,98
Flexibilität	%P/min	Max	20	20	100	100
Degradation	$\%_{\eta}$/1000h	Min	0,13	0,13	0,2	0,2
Produktreinheit	Vol.-%	Max	99,9	99,9	99,99	99,99
Flächenbedarf	m^2/MW	Min	63	63	14,48	14,48
CAPEX Elektrolyse	€/kW	Min	709	850	1363	1450
CAPEX H_2O Aufbereitung	€/kW	Min	6	6	4	4
CAPEX Verdichtung	€/kW	Min	62	9,1	62	9,1
CAPEX System	€/kW	Min	777	866	1429	1463
OPEX fix	€·(kW/a)$^{-1}$	Min	15,08	23,08	12,04	15,04
Energiebedarf Anlagenbau	kWh/kW	Min	5,74	5,74	7	7
Kritisches Material	kg/kW	Min	0	0	0,0006	0,0006
Wasserbedarf	l/kg	Min	15	15	10,6	10,6

Bei Betrachtung der Kriterienausprägungen des Energiebedarfs der Elektrolysesysteme wird deutlich, dass insbesondere die alkalische Druckelektrolyse deutlich höhere Werte aufweist, als die AEL mit atmosphärischem Betriebsdruck sowie beide PEMEL-Varianten (vgl. [19]). In einer durchgeführten Berechnung mit AspenPlus V11 wurden der jeweilige Energiebedarf und die CAPEX für die Verdichtung auf 75 bar berechnet. Aus dem aggregierten Kriterium Energiebedarf System wird ersichtlich, dass der deutlich geringere Energieaufwand für eine nachgeschaltete Verdichtung von 30 bar auf 75 bar bei der PEMEL Technologie zu einem Effizienzvorteil gegenüber der Variante bei atmosphärischem Betriebsdruck führt, während bei der AEL eine nachgeschaltete Verdichtung der LP

Ausführung vorteilhaft ist. Ebenfalls auf Basis einer Aspen Simulation wird der geringere Wasserbedarf der PEMEL im Betrachtungsfall 2 berechnet, welcher sich aus der Simulation einer Methanolsynthese mit dem zugehörigen Abwasserstrom und aus dem Verhältnis des Speisewasserwasserbedarfs der Elektrolyse ergibt. Auffällig ist der deutlich höhere Flächenbedarf für AEL, welcher um einen Faktor 4 größer als für PEMEL ausfällt [22]. Zudem ist die PEMEL Technologie deutlich flexibler im Betrieb und weist eine höhere Produktreinheit auf [20].[1] Demgegenüber findet bei der AEL eine deutlich langsamere Degradation der Stacks statt und die CAPEX sind in der LP Variante um etwa 46 % günstiger bzw. um 41 % in der HP Variante.

Für den Prozessschritt CO_2-Capture wird analog vorgegangen, wobei hier gemäß Abbildung 3 nur sechs Kriterien für die MCDA aufgegriffen werden. Unter den technischen Kriterien wird zwischen dem Flächenbedarf und dem Energiebedarf für die CO_2-Abscheidung unterschieden, wobei sich der Energiebedarf in einen thermischen und einen elektrischen Parameter unterteilt und zum Kriterium Energiebedarf System aggregiert wird. Die CAPEX werden für das CO_2-Capture und eine separate SO_2-Abscheidung aus dem Rauchgas des Kraftwerkes separat aufgeführt. Bezüglich der ökologischen Wirkungen wird der jeweils anfallende Aminbedarf berücksichtigt. Die zugrundeliegenden Parameter für die Kriterien sind in Tabelle 5 dargestellt.

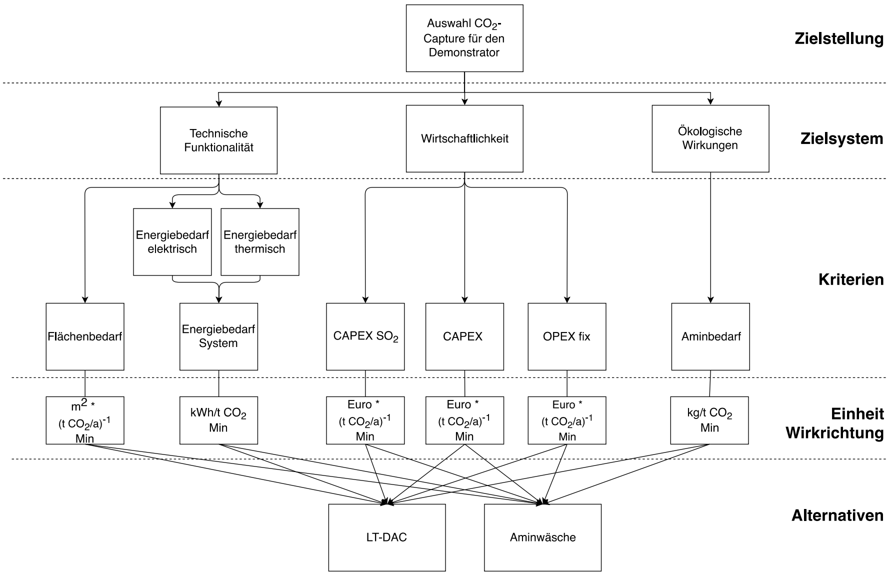

Abbildung 3: Darstellung der Kriterienhierarchie für den Prozessschritt CO2-Capture.

Die Energiebedarfe des LT-DAC wurden Fasihi et al. entnommen [9], während eine Prozesssimulation mit AspenPlus die Datenbasis für die Aminwäsche darstellt [3]. Die Simulation bildet den spezifischen Anwendungsfall „CO_2-Abscheidung aus dem Rauchgas der Raffinerie" ab und erlaubt über das Tool „Aspen Process Economic Analyzer" die Ermittlung der resultierenden CAPEX. Der Flächenbedarf für das LT-DAC fällt aufgrund der geringen CO_2-Konzentration in der Umgebungsluft deutlich größer aus, als für die Abscheidung aus dem KWK-Kraftwerk der Raffinerie (vgl. [27], [30]). Lediglich hinsichtlich der CAPEX für die Rauchgaswäsche zur Reduzierung des SO_2-Gehaltes ergibt sich ein Vorteil für das Direct Air Capture, da dieser Prozessschritt hier entfällt.

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[1] Parameter zur Flexibilität basierend auf vertraulichen Herstellerangaben.

Tabelle 5: Übersicht über die Parametrierung der berücksichtigten Kriterien für den Prozessschritt CO_2-Capture [9][31][27][32][33].

Kriterium / Alternative	**Einheit**	**Min/Max**	**LT-DAC**	**Aminwäsche**
Energiebedarf elektrisch	kWh_{el}/t_{CO2}	Min	250	12
Energiebedarf thermisch	kWh_{th}/t_{CO2}	Min	1750	1011
Energiebedarf System	kWh/t_{CO2}	Min	2000	1023
Flächenbedarf	$m^2 \cdot (t_{CO2}/a)^{-1}$	Min	0,1	0,01
CAPEX	$€ \cdot (t_{CO2}/a)^{-1}$	Min	598	123
CAPEX SO_2	$€ \cdot (t_{CO2}/a)^{-1}$	Min	0	12,89
OPEX fix	$€ \cdot (t_{CO2}/a)^{-1}$	Min	23,92	4,92
Aminbedarf	kg/t_{CO2}	Min	7,5	1,6

4. Ergebnisse und Diskussion

Gemäß der Saaty-Skala zur Gewichtung von Kriterien wurden jeweils für Elektrolyse und CO_2-Capture mittels des AHP Ansatzes eine paarweise Vergleichsmatrix aufgestellt und eine Kriteriengewichtung vorgenommen. Aus den jeweiligen Gewichtungen und den normalisierten Parametern kann schließlich eine Rangfolge gebildet werden, aus der sich eine Empfehlung für die Technologieauswahl ergibt. Die Ergebnisse werden im Folgenden diskutiert.

4.1 Ergebnisse für den Prozessschritt Elektrolyse

Die spezifischen Gewichtungen für alle Kriterien sind in Tabelle 6 dargestellt und ergeben sich aus der Umstellung der paarweisen Vergleichsmatrix aus Anhang A. Für den Prozessschritt Elektrolyse wurde unter den technischen Kriterien dem Energiebedarf eine besonders hohe Relevanz zugeordnet, da hieraus ein unmittelbarer Einfluss auf die Betriebskosten hervorgeht, welche wiederum entscheidend die Möglichkeit eines wirtschaftlichen Betriebs beeinflussen. Zudem ist ein geringerer Energiebedarf indirekt auch aus ökologischer Sicht zu favorisieren. Den Kriterien Flexibilität und Degradation wird eine vergleichsweise geringe Bedeutung beigemessen, da anzunehmen ist, dass sowohl für die AEL als auch PEMEL keine Einschränkungen in der Betriebsführung vorliegen. Den CAPEX wird die höchste Gewichtung zugeordnet, da diese einen zentralen Einfluss auf die Wirtschaftlichkeit ausüben. Für die Kriterien Degradation und Flächenbedarf ergibt sich eine mittlere Gewichtung, da hier ebenfalls deutliche Unterschiede auftreten. Die PEMEL kann aufgrund der höheren Zellstromdichte und vermindertem Peripherieaufwand wesentlich kompakter gebaut werden, weist allerdings eine stärkere Degradationsrate auf, was sich im Langzeitbetrieb wiederum negativ auf den Energiebedarf ausübt. Die erreichbare Produktreinheit wird für beide Technologien als ausreichend erachtet und erhält daher eine niedrige Gewichtung. Der Wasserbedarf ist von höherer Bedeutung, da dieser generell zwar für beide Technologieoptionen als gleich hoch anzusetzen ist, in der Unterscheidung der zwei Betrachtungsfälle jedoch von zentraler Relevanz ist.

Tabelle 6: Gewichtung der Kriterien für die Auswahl eines Elektrolyseurs.

Energiebedarf System	**Flexibilität**	**Degradation**	**Produktreinheit**	**Flächenbedarf**	**CAPEX System**	**OPEX fix**	**Energiebedarf Anlagenbau**	**Krit. Material**	**Wasserbedarf**
22 %	5 %	10 %	4 %	11 %	25 %	9 %	2 %	2 %	9 %

Zur Überprüfung der Konsistenz der paarweisen Vergleiche wurde der maximale Eigenwert $\lambda_{max} = 10{,}91$ berechnet und gemäß Gleichung 5 in den Konsistenzindex $CI = 0{,}10$ überführt. Auf Basis des Zufallsindex $RI = 1{,}49$ und Gleichung 6 ergibt sich ein zulässiges Konsistenzverhältnis von $CR = 0{,}068$.

Für beide Betrachtungsfälle wird auf Basis der gewichteten Kriterien und einer in Abhängigkeit der Wirkrichtung der Kriterienausprägungen durchgeführten linearen Normalisierung (vgl. Anhang B) separat unter Anwendung der Nutzwertanalyse eine Rangfolge gebildet.

Tabelle 7: Berechnete Rangfolge der vier bewerteten Alternativen für beide Betrachtungsfälle.

	Betrachtungsfall 1		**Betrachtungsfall 2**	
Alternative	**Nutzwert**	**Rangfolge**	**Nutzwert**	**Rangfolge**
AEL atm	0,8471	1	0,8471	2
AEL 30 bar	0,7692	4	0,7692	4
PEMEL atm	0,8086	2	0,8484	1
PEMEL 30 bar	0,7917	3	0,8316	3

In Tabelle 7 sind die berechneten Nutzwerte für die untersuchten Betrachtungsfälle dargestellt. In der Rangfolge erzielt die alkalische Elektrolyse bei atmosphärischem Betriebsdruck den höchsten Nutzwert im Betrachtungsfall 1. Aufgrund der deutlichen Vorteile dieser Alternative in den am höchsten gewichteten Kriterien Energiebedarf und CAPEX kann das Ergebnis als plausibel erachtet werden. Die beiden Ausführungen der PEM-Elektrolyse erzielen insbesondere aufgrund ihrer Vorteile bezüglich des Flächenbedarfs und der Wartungskosten die Ränge 2 und 3. Den niedrigsten Nutzwert erzielt die alkalische Druckelektrolyse, da diese einen deutlich geringeren Wirkungsgrad als die übrigen Alternativen aufweist.

In Betrachtungsfall 2 schneidet die atmosphärische PEM-Elektrolyse am besten ab, da der deutlich reduzierte Wasserbedarf sich zusätzlich sowohl auf das Kriterium Energiebedarf, als auch geringfügig auf die CAPEX positiv auswirkt. Bei einer zu erwartenden Reduktion der CAPEX in den kommenden Jahren könnte die PEM-Elektrolyse für die Prozesskette Power-to-Methanol deutliche Vorteile aufweisen, vorausgesetzt, eine Wasserrückführung aus der Methanolsynthese ist auch im realen Betrieb möglich. Da hier noch keine Erfahrungswerte vorliegen, kann über die Möglichkeit der Umsetzung einer solchen Prozesskette noch keine validierte Aussage getroffen werden.

4.2 Ergebnisse für den Prozessschritt CO_2-Capture

Analog zur Kriteriengewichtung für die Elektrolyse wurden auch für die Auswahl der CO_2-Capture Technologie der benötigte Energiebedarf und die Investitionskosten als besonders relevant bewertet. Als Ergebnis der paarweisen Vergleichsmatrix (vgl. Anhang C) wurden zudem dem Flächen- und Aminbedarf zur CO_2-Abscheidung eine mittlere Bedeutung zugeordnet. Die Investitionskosten für die SO_2-Abscheidung aus dem Rauchgasstrom des Kraftwerkes sowie die Wartungskosten für beide Technologien wurden als weniger relevant bewertet und erzielen eine geringe Gewichtung von 5-6 %.

Tabelle 8: Gewichtung der Kriterien zur Technologieauswahl für das CO2-Capture.

Energiebedarf System	**Flächenbedarf**	**CAPEX**	**CAPEX SO_2**	**OPEX fix**	**Aminbedarf**
32 %	13 %	32 %	5 %	6 %	13 %

Aus der Konsistenzüberprüfung mit $\lambda_{max} = 6{,}08$ und einem Konsistenzindex von $CI = 0{,}02$ ergibt sich mit einem bei sechs Kriterien gültigen Zufallsindex von $RI = 1{,}24$ ein zulässiges Konsistenzverhältnis von $CR = 0{,}014$.

Die normalisierten Kriterienausprägungen zur Bildung einer Rangfolge sind in Anhang D dargestellt. Aus Tabelle 9 gehen die Berechnungsergebnisse aus der Nutzwertanalyse hervor. Die CO_2-Abscheidung aus dem Rauchgasstrom des KWK-Kraftwerks mittels Aminwäsche schneidet deutlich besser als das Direct Air Capture ab. Das Ergebnis fällt mit Blick auf die Kriterienausprägungen nicht überraschend aus, da die CO_2-Abscheidung aus einer Punktquelle deutlich effizienter und kostengünstiger darstellbar ist. Bei der Deutung der erzielten Ergebnisse gilt es jedoch stets zu berücksichtigen, dass die zugrundeliegenden Umweltwirkungen eingehender Energie- und Stoffströme nicht zur Bewertung der jeweiligen Einzeltechnologien herangezogen wurden. Folglich ist der fossile Ursprung des aus dem Kraftwerk abgeschiedenen CO_2 nicht in die Bewertung eingeflossen. Diesbezüglich ist eine sachgemäße Allokation der durch das Kraftwerk verursachten Emissionen sicherzustellen, so dass diese weiterhin dem Kraftwerk bzw. Strom und Prozesswärme und/oder dem produzierten Methanol zugeordnet werden [34].

Tabelle 9: Berechnete Nutzwerte und Rangfolge.

Alternative	Nutzwert	Rangfolge
LT-DAC	0,3326	2
Aminwäsche	0,9600	1

5. Zusammenfassung

Die Erzeugung strombasierter, synthetischer Kraftstoffe und Basischemikalien durch sogenannte Power-to-X Konzepte stellt einen vielversprechenden Ansatz zur Reduzierung von Treibhausgasemissionen und zur Kopplung der Sektoren Strom, Wärme, Verkehr und Industrie dar. Die zugrundeliegenden Technologien solcher Prozessketten sind bereits grundsätzlich bekannt und unterschiedlich weit entwickelt. Im Rahmen dieser Ausarbeitung wurde eine Technologieempfehlung für Prozessschritte Elektrolyse und CO_2-Capture einer Power-to-Methanol Anlage am Standort der Raffinerie Heide auf Basis einer multikriteriellen Analyse erarbeitet. Die Bewertung wurde unter Berücksichtigung spezifischer technischer, wirtschaftlicher und ökologischer Kriterien und unter Anwendung der Methoden des AHP und der Nutzwertanalyse durchgeführt, wobei das vorgestellte methodische Vorgehen, die Kriterienauswahl sowie die Kriterienparametrierung als Ausgangspunkt für weitere PtX-Fallstudien herangezogen werden können.

Für den Prozessschritt Elektrolyse wurden die AEL und PEMEL Technologie jeweils für den Betrieb bei atmosphärischem Druck (LP) sowie bei einem Betriebsdruck von 30 bar (HP) verglichen. Die AEL bei atmosphärischem Betriebsdruck erzielte den höchsten Nutzwert und weist insbesondere in den Kriterien Energiebedarf und CAPEX deutliche Vorteile gegenüber den übrigen Alternativen auf. Demgegenüber erzielte die alkalische Druckelektrolyse insbesondere aufgrund eines sehr hohen spezifischen Energiebedarfs den geringsten Nutzwert. Die beiden PEMEL Varianten erzielten vergleichbare Ergebnisse und schnitten in der Rangfolge auf Rang 2 (PEMEL LP) und Rang 3 (PEMEL HP) ab. In der Literatur wird zudem eine Besonderheit der PEMEL diskutiert, auch mit Methanol verunreinigtes Wasser verarbeiten zu können. Diese Option könnte im Rahmen einer Power-to-Methanol Anlage besonders attraktiv sein, da somit der Abwasserstrom aus der Methanolsynthese ohne weitere Aufbereitung zur Elektrolyse zurückgeführt und die energieintensive Wasseraufbereitung von

Frischwasser anteilig reduziert werden kann. In einem zweiten Betrachtungsfall wurde daher angenommen, dass der Abwasserstrom der Methanolsynthese für die PEM-Elektrolyse genutzt kann. In diesem Betrachtungsfall konnte die PEMEL (LP) trotz der deutlich höheren CAPEX den höchsten Nutzwert erzielen, gefolgt von der AEL (LP), PEMEL (HP) und AEL (HP).

Bei der Bewertung von CO_2-Capture Technologien wurden das Direct Air Capture Verfahren von Climeworks, das mit Niedertemperaturwärme betrieben wird, sowie die etablierte Technologie der Aminwäsche zur Abscheidung von CO_2 aus dem KWK-Kraftwerk der Raffinerie Heide bewertet. Die Aminwäsche erzielte den deutlich höheren Nutzwert, da die CO_2-Abscheidung aus einer Punktquelle deutlich effizienter und kostengünstiger darstellbar ist als eine Abscheidung aus der Umgebungsluft. Es ist jedoch zu beachten, dass der abweichende Ursprung des CO_2 nicht in die ausgeführte Bewertung eingeflossen ist.

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Anhang

A:

Paarweise Vergleichsmatrix der Kriterien zur Bewertung der Elektrolyse-Alternativen.

	Energiebedarf System	**Flexibilität**	**Degradation**	**Produktreinheit**	**CAPEX System**	**OPEX fix**	**Flächenbedarf**	**Energiebedarf Anlagenbau**	**Krit. Material**	**Wasserbedarf**
Energiebedarf System	1,00	5,00	3,00	5,00	1,00	3,00	3,00	7,00	7,00	3,00
Flexibilität	0,20	1,00	0,33	1,00	0,20	0,33	0,33	5,00	5,00	0,33
Degradation	0,33	3,00	1,00	3,00	0,33	1,00	1,00	5,00	5,00	1,00
Produktreinheit	0,20	1,00	0,33	1,00	0,20	0,20	0,20	3,00	3,00	0,33
CAPEX System	1,00	7,00	3,00	7,00	1,00	5,00	3,00	7,00	7,00	3,00
OPEX fix	0,33	5,00	1,00	5,00	0,33	1,00	0,20	3,00	3,00	1,00
Flächenbedarf	0,33	5,00	1,00	5,00	0,33	1,00	1,00	5,00	5,00	1,00
Energiebedarf Anlagenbau	0,14	0,33	0,20	0,33	0,14	0,33	0,20	1,00	1,00	0,33
Krit. Material	0,14	0,33	0,20	0,33	0,14	0,33	0,20	1,00	1,00	0,33
Wasserbedarf	0,33	3,00	1,00	3,00	0,33	1,00	1,00	3,00	3,00	1,00

B:

Transponierte Kriterienausprägungen als Grundlage für eine dimensionslose Vergleichbarkeit der Elektrolyse-Alternativen.

Kriterium/ Alternative	**Energiebedarf System**	**Flexibilität**	**Degradation**	**Produktreinheit**	**Flächenbedarf**	**CAPEX System**	**OPEX fix**	**Energiebedarf Anlagenbau**	**Kritisches Material**	**Wasserbedarf**
Einheit	**kWh/Nm^3**	**%P/min**	**%$_\eta$/1000h**	**Vol.-%**	**m^2/MW**	**€/kW**	**€·(kW/a)$^{-1}$**	**kWh/kW**	**kg/kW**	**Liter/kg**
Min/Max	**Min**	**Max**	**Min**	**Max**	**Min**	**Min**	**Min**	**Min**	**Min**	**Min**
AEL atm	1,0000	0,2000	1,0000	0,9991	0,2298	1,0000	0,7983	1,0000	1,0000	1,0000
AEL 30 bar	0,8757	0,2000	1,0000	0,9991	0,2298	0,8973	0,5217	1,0000	1,0000	1,0000
PEMEL atm	0,9610	1,0000	0,6500	1,0000	1,0000	0,5430	1,0000	0,8200	0,0000	1,0000
PEMEL 30 bar	0,9801	1,0000	0,6500	1,0000	1,0000	0,5303	0,8006	0,8200	0,0000	1,0000

C:

Paarweise Vergleichsmatrix der Kriterien zur Bewertung der CO_2-Capture Alternativen.

	Energiebedarf System	**Flächenbedarf**	**CAPEX**	**CAPEX SO2**	**OPEX fix**	**Aminbedarf**
Energiebedarf System	1,00	3,00	1,00	5,00	5,00	3,00
Flächenbedarf	0,33	1,00	0,33	3,00	3,00	1,00
CAPEX	1,00	3,00	1,00	5,00	5,00	3,00
CAPEX SO2	0,20	0,33	0,20	1,00	0,33	0,33
OPEX fix	0,33	0,33	0,20	1,00	1,00	0,33
Aminbedarf	0,33	1,00	0,33	3,00	3,00	1,00

D:

Transponierte Kriterienausprägungen als Grundlage für eine dimensionslose Vergleichbarkeit der CO_2-Capture Alternativen.

Kriterium/ Alternative	**Energiebedarf System**	**Flächenbedarf**	**CAPEX**	**CAPEX SO_2**	**OPEX fix**	**Aminbedarf**
Einheit	**kWh/t_{CO2}**	**$m^2\cdot(t_{CO2}/a)^{-1}$**	**$€\cdot(t_{CO2}/a)^{-1}$**	**$€\cdot(t_{CO2}/a)^{-1}$**	**$€\cdot(t_{CO2}/a)^{-1}$**	**kg/t_{CO2}**
Min/Max	**Min**	**Min**	**Min**	**Min**	**Min**	**Min**
LT-DAC	0,51150	0,10000	0,20569	1,00000	0,20569	0,21333
Aminwäsche	1,00000	1,00000	1,00000	0,00000	1,00000	1,00000

Ausgewählte Standortfaktoren für Power-to-Fuel-Anlagen: Erdölraffinerie versus grüne Wiese

Christian Schnülle, Timo Wassermann, Michael Kalis und Judith Schäfer

Sog. Power-to-X (PtX)- bzw. Power-to-Fuel (PtF)-Konzepte gelten als Schlüssel zur Defossilisierung des Schiffs-, Flug- und Schwerlastverkehrs und vieler Industrieprozesse. In Bezug auf die Standortwahl für PtF-Anlagen kann zwischen Ansätzen zur Integration in die Bestandsindustrie und Vorhaben auf „der grünen Wiese“ unterschieden werden. In diesem Artikel werden ausgewählte Standortfaktoren der beiden Ansätze aus ökonomischer und regulatorischer Perspektive beleuchtet.

Wasserstoff aus Wasser-Elektrolyse, welche mit erneuerbarem Strom betrieben wird, kann entweder direkt genutzt oder mit abgeschiedenem CO_2 zu langkettigen Kohlenwasserstoffen umgesetzt werden. Diese können auf fossiler Basis hergestellte Chemikalien oder Kraftstoffe eins-zu-eins substituieren. Für einen zügigen Markthochlauf müssen besonders vorteilhafte Bedingungen für die Errichtung und den Betrieb entsprechender Anlagen identifiziert bzw. etabliert werden. Diese werden im Folgenden in wirtschaftlicher und rechtlicher Hinsicht dargestellt und analysiert (vgl. Abb. 1).

Regulatorische Aspekte der Genehmigungsphase: Bau- und immissionsschutzrechtliche Einordnung

Die Errichtung eines Elektrolyseurs bedarf nach der überwiegenden Behördenpraxis einer immissionsschutzrechtlichen Genehmigung. Das Bundes-Immissionsschutzgesetz normiert für Anlagen, die ein gewisses Immissionspotenzial aufweisen, eine Genehmigungspflicht [1]. Nach Ansicht der Behörden sind Elektrolyseure unter den Genehmigungstatbestand für Anlagen zu fassen, die Gase, wie Wasserstoff, durch chemische, biochemische und biologische Umwandlung in industriellem Umfang herstellen [2]. Der Begriff des „industriellen Umfangs“ schließt eine Anwendung auf Kleinanlagen keineswegs aus [3]. In der Regel wird ein industrieller Umfang bei einer Herstellung des Produkts zu gewerblichen Zwecken angenommen [4]. Dezentrale Kleinanlagen im Sinne eines grüne-Wiese-Ansatzes und großskalige Industrieanlagen werden somit unterschiedslos behandelt und stehen vor den gleichen bürokratischen Hürden sowie Kostenfragen im Rahmen der Genehmigungspraxis [5].

Doch auch wenn man eine Genehmigungsbedürftigkeit für Elektrolyseure mangels industriellen Umfangs bestreitet, kann sich regelmäßig ein immissionsschutzrechtliches Verfahren wegen der Lagerung von Wasserstoff aufdrängen. Bereits bei einer Lagerung von 3 bis maximal 30 t ist ein Verfahren durchzuführen [6]. Diese Mengenschwellen können bereits durch Kleinanlagen erreicht werden [7].

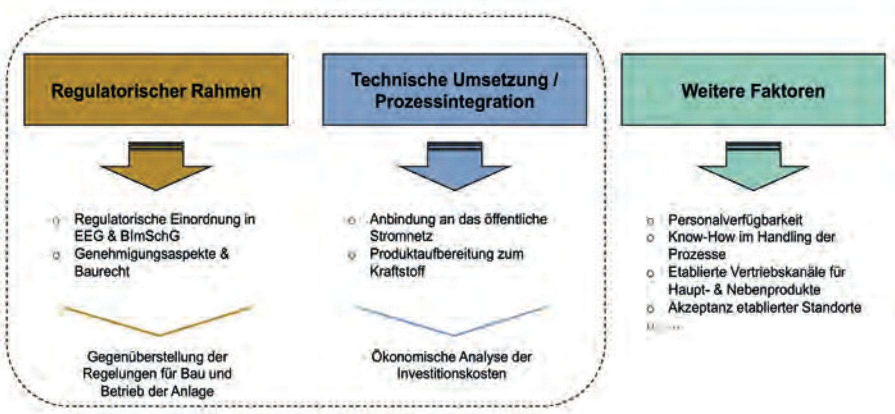

Abb. 1 Darstellung identifizierter Standortfaktoren für die Gegenüberstellung der Ansätze „Integration in Erdölraffinerien“ und „grüne Wiese“

Baurechtlich ist zwischen Planbereich, Innenbereich und Außenbereich zu unterschieden [8]. Soll der Elektrolyseur auf der grünen Wiese außerhalb einer Gemeinde errichtet werden, dann handelt es sich typischerweise um den Außenbereich [9]. Dieser ist grundsätzlich von Bebauung freizuhalten, sofern diese nicht typischerweise in den Außenbereich gehört. Das Gesetz unterscheidet zwischen privilegierten und sonstigen, nicht privilegierten Vorhaben [10]. Letztere müssen deutlich strengere Anforderungen erfüllen. Elektrolyseure könnten als standortgebundene Infrastruktureinrichtungen privilegiert sein [11]. Dafür müssten sie der öffentlichen Versorgung mit Elektrizität oder Gas dienen und eine Ortsgebundenheit aufweisen.

Ortsgebundenheit setzt eine räumliche Beziehung voraus, auf die das Vorhaben angewiesen ist, die sich auf eine näher eingrenzbare Stelle im Außenbereich bezieht [12]. Das Vorhaben darf nicht beliebig an anderer Stelle im Außenbereich errichtet werden können. Ortsgebundenheit könnte vorliegen, wenn der Elektrolyseur aufgrund einer Direktleitung und des Grünstrombezugs auf die Nähe zu EE-Anlagen angewiesen ist [13]. Gegebenenfalls genügt auch der netzstabilisierende Einsatz des Elektrolyseurs als Speicher [14]. Privilegiert sind auch Vorhaben, die der Erforschung, Entwicklung oder Nutzung der Windenergie dienen. Dienen setzt voraus, dass der Elektrolyseur der EE-Anlage funktional unmittelbar zu- und untergeordnet ist [15]. Dies kann erfüllt sein, wenn der Elektrolyseur als Speicher fungiert und das Ziel hat, Stromüberschüsse zur Vermeidung von Abregelungen aus den EE-Anlagen aufzunehmen. Im Hinblick auf die benötigte Volllaststundenzahl zur Sicherstellung eines rentablen Anlagenbetriebs sind diese Voraussetzungen nicht unproblematisch.

In der Bestandsindustrie ist die Genehmigung ungleich einfacher. Maßgeblich sind die Festsetzungen des Bebauungsplans oder die faktischen Gegebenheiten im unbeplanten Innenbereich [16]. Wenn in dem betreffenden Gebiet bereits industrielle Anlagen angesiedelt sind, wird es sich in der Regel um ein Gewerbegebiet oder ein Industriegebiet handeln [17]. Dort können ELY entweder als Gewerbebetriebe oder als untergeordnete Nebenanlagen zugelassen werden [18]. Eine untergeordnete Nebenanlage dient der Hauptanlage in funktioneller und räumlich gegenständlicher Weise [19]. Dies setzt ein Mindestmaß an Zusammengehörigkeit zwischen Haupt- und Nebenanlage voraus [20], was typischerweise bei der Einbindung eines Elektrolyseurs in eine industrielle Anlage der Fall sein wird. Die Genehmigungsvoraussetzungen für Elektrolyseure in industriellen Anlagen sind damit aufgrund der bereits bestehenden industriellen Bebauung ungleich geringer als bei einer Errichtung auch kleinerer Anlagen im Außenbereich. Für den unbeplanten Innenbereich gilt dasselbe, wenn ein faktisches Gewerbe- oder Industriegebiet vorliegt.

Regulatorische Aspekte der Betriebsphase: Strompreisbestandteile

Die staatlich veranlassten Strompreisbestandteile können mittlerweile über 70 % des Strompreises ausmachen [21]. Damit ist der Strompreis für den Betrieb der Elektrolyse der maßgebliche Kostenfaktor. Vor diesem Hintergrund ist es für Betreiber von Elektrolyseuren entscheidend, ob und inwieweit die staatlich veranlassten Strompreisbestandteile vermieden, also Privilegierungen und Befreiungen in Anspruch genommen werden können. Die Strompreisbestandteile, bestehend aus Stromsteuer, Netzentgelten, netzentgeltgekoppelten Umlagen und EEG-Umlage, fallen beim Betrieb von Elektrolyseuren, die als sog. Letztverbraucher eingeordnet werden [22], grundsätzlich in voller Höhe an. Unterschiedslos wirken die befristete Befreiung von den (Strom-) Netzentgelten für Elektrolyseure [23] sowie der Steuererlass für Strom, der nachweislich für die Elektrolyse eingesetzt wird [24]. Für Industrieanlagen kann ein weiterer Steuererlass im Falle der Energieintensität infrage kommen [25]. Demgegenüber könnten grüne-Wiese-Ansätze von einer Steuerbefreiung für im räumlichen Zusammenhang bezogenen EE-Strom profitieren, da die elektrische Nennleistung der EE-Anlage hier auf 2 MW beschränkt ist [26].

Wesentlicher Treiber für eine unterschiedliche Behandlung von Anlagen in der Bestandsindustrie und grüne-Wiese-Ansätzen bleibt damit die EEG-Umlage. Diese fällt zunächst grundsätzlich in voller Höhe an [27]. Von Stakeholdern und Politik wird regelmäßig die Besondere Ausgleichsregelung für stromkostenintensive Unternehmen als wesentlicher Befreiungstatbestand herangezogen [28]. Auf Antrag wird die EEG-Umlage auf 15 % begrenzt [29], wovon die erste Gigawattstunde allerdings ausgenommen ist [30]. Das führt dazu, dass kleinere Anlagen regelmäßig nicht von der Begrenzung profitieren. Unbeschadet dessen war die Anwendung der Besonderen Ausgleichsregelung für Elektrolyseure kein Regelfall. Die Privilegierung greift nur für Unternehmen, die sich einer bestimmten Branche zuordnen lassen [31]. Die Herstellung von Wasserstoff ist dabei nicht ausdrücklich adressiert, jedoch die Mineralölverarbeitung [32]. So könnte etwa eine Anlage zur Mineralölverarbeitung einen Elektrolyseur und damit die Wasserstoffproduktion in ihr Portfolio aufnehmen und gleichzeitig als einschlägige Branche von der Begrenzung der EEG-Umlage profitieren.

Mit der EEG-Novelle 2021 wurde eine Anwendung der Besonderen Ausgleichsregelung auf (alleinstehende) Elektrolyseure unabhängig von der anschließenden Verwendung des Wasserstoffs eingeführt [33]. Für diese ist auch keine Begrenzung der EEG-Umlage für die erste Gigawattstunde vorgesehen. Die Elektrolyse muss jedoch den größten Wertschöpfungsbeitrag des Unternehmens leisten [34], sodass eine Anwendung der Regelung auf PtF-Anlagen regelmäßig ausscheiden wird. Letztlich können damit sowohl industrielle als auch grüne Wiese-Ansätze von einer Reduzierung der EEG-Umlage profitieren. Für Letztere mag sich jedoch aufgrund der Begrenzung für den gesamten bezogenen Strom eine Beschränkung auf die Elektrolyse aufdrängen.

Analyse der Investitionskosten für PtF-Anlagen

Die Analyse ausgewählter Investitionskostenbestandteile wird exemplarisch für eine PtF-Anlage mit 50 MW Elektrolyse-Eingangsleistung dargestellt. Kasten et al. haben diese Anlagengröße, abgesehen von dezentralen (Container-)lösungen, als Mindestgröße für Fischer-Tropsch (FT) PtF-Anlagen identifiziert [35]. Neben einer Analyse der Investitionssummen für verschiedene Aufbereitungsintensitäten des FT-Rohölsubstituts („SynCrude“) werden zusätzliche Kosten für den Anschluss an das öffentliche Stromnetz betrachtet. Dabei orientiert sich die Technologieauswahl vorrangig am Technology Readiness Level (TRL). So werden die alkalische Elektrolyse (AEL) zur Wasserstoff-

	Investitionssumme in Mio. €		
	Anlage zur Produktion von SynCrude	Anlage inkl. Teil-Raffination	Anlage inkl. vollumfänglicher Raffination
AEL	39,0	39,0	39,0
Aminwäsche	16,3	16,3	16,3
FT-Synthese inkl. RWGS-Reaktor	27,9	27,9	27,9
Destillationskolonne, Wachs-Hydrocracker	-	17,4	17,4
Hydrotreater Mitteldestillat, Hydrotreater Naphta, Katalytischer Reformer, C5/C6-Isomerisierung	-	-	26,4
Summe	**83,2**	**100,6**	**127,0**

Tab. **Aufstellung der Investitionskosten für verschiedene Aufbereitungsintensitäten**

bereitstellung, die Aminwäsche zur CO_2-Abscheidung aus einer Punktquelle und die FT-Synthese zur eigentlichen Kraftstoffsynthese betrachtet.

PtF-Anlageninvestition

Für den Elektrolyseur werden gemäß Proost et al. ein Energiebedarf von 4,8 kWh/Nm^3_{H2} sowie skalierungsspezifische Systemkosten von 506 €/kW angesetzt [36]. Damit belaufen sich die „nackten“ Anschaffungskosten auf 25,3 Mio. € und resultieren, unter Berücksichtigung eines reduzierten Lang-Faktors, in einer Investitionssumme (Fixed Capital Investment, FCI) von 39,0 Mio. € [37].

Die Dimensionierung der Aminwäsche und FT-Synthese erlaubt die Verarbeitung des erzeugten Wasserstoffs, wobei für alle Anlagenteile 8.000 Volllaststunden pro Jahr angenommen werden. Die Aminwäsche wird auf Basis einer AspenPlus-Simulation angenähert (vgl. [38]) und beläuft sich auf ein FCI in Höhe von 16,3 Mio. €. Der vorgeschaltete RWGS- sowie der eigentliche FT-Reaktor begründen FCI in Höhe von 27,9 Mio. € und verfügen über eine jährliche Produktionskapazität von 13.670 t flüssiger Kohlenwasserstoffe. Bei dem zugrunde gelegten FT-Konzept nach [39] handelt es sich um eine Niedertemperatursynthese mit Co-Katalysator, die u.a. zur Herstellung von Kerosin und Diesel geeignet ist.

PtF-Prozessketten werden in Studien häufig nur bis zur Synthese bzw. im Falle der FT-Route bis zum SynCrude beschrieben. Zur Herstellung spezifikationsgerechter Produkte, wie Drop-in Kraftstoffe oder Basischemikalien, ist jedoch eine Aufbereitung des SynCrudes notwendig, da es über ein breites Spektrum an Kohlenwasserstoffen unterschiedlicher Kettenlängen verfügt. Dies schließt eine Destillation und weitere Schritte wie Hydrotreating, Hydrocracking, katalytische Isomerisierung und Reformierung ein [40].

Während die verschiedenen Verfahren zur Raffination von Erdöl bzw. SynCrude in einer Erdölraffinerie bereits vorhanden sind, ist der Aufbau sämtlicher Teilanlagen auf der „grünen Wiese“ mit erheblichem Mehraufwand verbunden. Zwar ist ein Vertrieb des Erdölsubstituts an etablierte Erdölraffinerien zur dortigen Weiterverarbeitung möglich. Im Sinne eines dezentralen Ansatzes zur Herstellung von synthetischen Kraftstoffen wird dennoch eine Teil-Raffination inklusive Destillation und Hydrocracking als Bestandteil der PtF-Anlage mitbetrachtet. Für eine gänzlich dezentrale FT-Raffination werden zudem alle weiteren Prozessschritte gemäß der Tabelle berücksichtigt.

Für die Prozessintegration in eine Erdölraffinerie und Beimischung des SynCrudes zum Rohöl (Co-Processing) ergibt sich demnach eine Investitionssumme von 83,2 Mio. €. Wird eine Umsetzung auf der grünen Wiese angestrebt, erhöht sich diese bei Teil- oder vollständiger Raffination des SynCrudes auf 100,6 bzw. 127 Mio. €. Dies entspricht einem um 62 % bzw. 157 % erhöhten Investitionsbedarf für die FT-Teilanlage.

Stromanschlusskosten

Je nach Größe der Anlage bzw. des Elektrolyseurs variieren die Investitionen für einen Stromanschluss erheblich. Für Anlagen mit einer elektrischen Eingangsleistung im mittleren zweistelligen MW-Bereich wird ein Anschluss an das Hochspannungsnetz benötigt. Für die Errichtung eines neuen Umspannwerkes mit einem Transformator inklusive eines 110 kV- und eines 20-kV-Schaltfelds können nach [41] etwa 2,0 Mio. € exklusive weiterer Kosten für Grundstücke, Gebäude und die Verlegung von Kabeln bzw. Leitungen veranschlagt werden. Aus einer internationalen Studie zur Erhebung der Kosten für Stromversorgungsinfrastrukturen in Europa resultieren für ein 110-kV-Umspannwerk Kosten in Höhe von 4,7 Mio. € [42].

Die Spannweite der Kosten für die Verlegung von Erdkabeln zwischen 110-150 kV fällt mit Literaturangaben von 390.000-816.000 €/km relativ groß aus. Für ein 110-kV-Einfach-Freileitungssystem ergeben sich 220.000 €/km [43, 44]. Bei einer angenommenen Strecke von 10 km resultieren aus einer unterirdischen Verlegung von Kabeln demnach Kosten in Höhe von 3,9-8,2 Mio. €. Für ein Einfach-Freileitungssystem entstehen Kosten von 2,2 Mio. €.

Für den hier zugrundeliegenden Betrachtungsfall einer 50 MW_{el}-Anlage und 10 km Strecke bis zum nächsten Netzanknüpfungspunkt resultieren Gesamtinvestitionen in Höhe von 6,9-12,9 Mio. €, die bei einer bereits ausreichend gegebenen infrastrukturellen Anbindung entfallen. Die Stromanschlusskosten betragen somit bis zu 9,4 % des identifizierten Anlageninvests.

Abb. 2 stellt die Investitionen für beide Grenzfälle gegenüber: 1) Co-Processing in Erdölraffinerie bei bereits ausreichender Anbindung an das Stromnetz und 2) PtF-Anlage mit vollständiger Raffination auf der grünen Wiese. Die Anlageninvestitionen sind bei Co-Processing in einer Raffinerie um 39,2 % geringer.

Diskussion der Ergebnisse aus regulatorischer und ökonomischer Perspektive

Aus ökonomischer Perspektive scheint die Option einer Prozessintegration in Erdölraffinerien aufgrund der zunächst deutlich

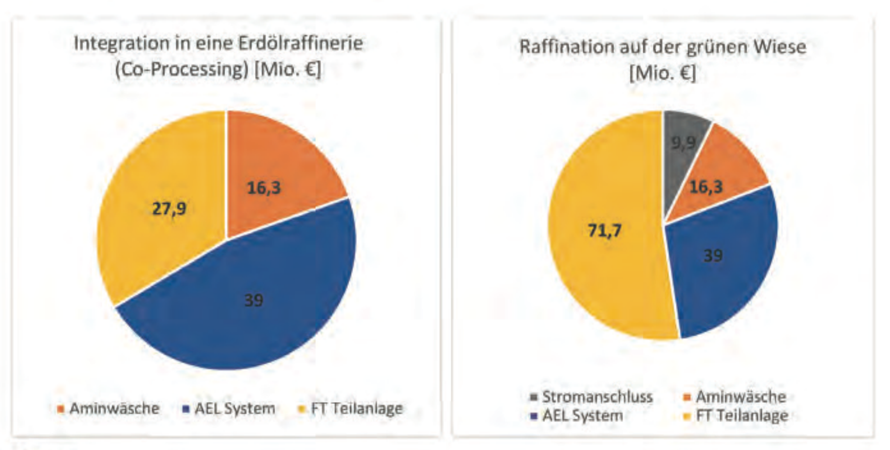

Abb. 2 **Aufstellung der Investitionssummen unter den getroffenen Annahmen für die Ansätze „Integration in eine Erdölraffinerie“ und „grüne Wiese“**

geringeren Investitionskosten vorerst attraktiver als die Umsetzung neuer Vorhaben auf der grünen Wiese. Durch eine potenziell ausreichende Anbindung an das Stromnetz und die Möglichkeit des Co-Processings können deutliche Einsparungen in der Umsetzung einer PtF-Anlage erzielt werden. Auch aus regulatorischer Sicht ist die Integration und damit Errichtung einer Nebenanlage in eine bestehende Industrieanlage erleichtert. Die immissionsschutzrechtliche Genehmigungsbedürftigkeit steht dem nicht entgegen und stellt für Betreiber von Industrieanlagen wohl kaum ein wesentliches Hemmnis dar. Die im Wesentlichen unterschiedslose Berücksichtigung bei den Strombezugskosten begründet keine abweichende Einschätzung.

Die Beimischung von SynCrude in der konventionellen Rohölverarbeitung kann gemäß [45] aufgrund abweichender Produktspezifikationen allerdings nicht uneingeschränkt erfolgen und ist somit als Zwischenschritt einer Transformation von Erdölraffinerien zu verstehen. Auch im Kontext globaler Klimaschutzziele kann ein Co-Processing nur kurz- bis mittelfristig als zielführend erachtet werden. Dies müsste mit einem graduellen Aufbau der Kapazitäten für synthetische Produkte bei gleichzeitiger Reduktion der Rohölverarbeitung einhergehen, womit wiederum eine Transformation der Kraftstoffaufbereitungsinfrastrukturen verbunden wäre. Die Option des Co-Processings stellt damit vielmehr einen möglichen ersten Schritt für die Markteinführung synthethischer, strombasierter Kraftstoffe als „Blend-Kraftstoff“ dar.

In diesem Zusammenhang sind deshalb auch grüne-Wiese-Ansätze für die Forcierung eines Markthochlaufs erforderlich. Hier könnten kurzfristig vor allem kleinskalige, modulare Konzepte Vorteile bieten, wie sie bereits in Demonstrationsprojekten umgesetzt werden. Unbeschadet dessen kann auch eine Produktion der Zwischenprodukte für die ausschließlich auf erneuerbaren Energien beruhenden strombasierten, synthetischen Kraftstoffe für Kleinanlagen von Relevanz sein. Hier kann die EEG-Umlagereduzierung für die Herstellung von Wasserstoff ohne den sonst anfallenden Selbstbehalt für die erste GWh als Anreiz wirken. Diese dezentralen Ansätze werden durch die immissionsschutzrechtliche Gleichbehandlung von Kleinanlagen und Industrieanlagen jedoch eingeschränkt.

Anmerkungen

[1] §§ 4 ff BImSchG.

[2] § 4 BImSchG i.V.m. Nr. 4.1.12 Anhang 1 der 4. BImSchV. Diese Genehmigungspraxis wird teilweise mit Verweis darauf abgewiesen, dass es sich bei der Elektrolyse um eine elektrolytische statt chemische Umwandlung handele, vgl. Bringewat, J.: Rechtsfragen bei der Zulassung von Elektrolyseurprojekten. JurOP 2017 online abrufbar unter: http://www.jurop.org/oeffbaurecht/aktuelle-rechtsfragen-bei-der-zulassung-von-elektrolyseurprojekten/ (zuletzt abgerufen am 10.12.2020).

[3] Siehe zum Begriff auch die Grundsätze zur Bestimmung des Begriffs der „fabrikmäßigen Herstellung“ der Bund-Länderarbeitsgemeinschaft, Länderausschuss für Immissionsschutz Verwaltungsvorschriften zur 4. BImSchV S. 25, Nr. 4.1.

[4] Europäische Kommission: Frequently Asked Questions (FAQ) – Industrial Emissions Directive (IED) 2010/75/EU, abrufbar unter: https://ec.europa.eu/environment/industry/stationary/ied/faq.htm (zuletzt abgerufen am 10.12.2020).

[5] Ein vereinfachtes Genehmigungsverfahren ohne Öffentlichkeitsbeteiligung wäre für Elektrolyseure eröffnet, wenn diese als Biogasanlagen eingeordnet würden, § 4 BImSchG i.V.m. Nr. 1.15 Anhang 1 der 4. BImSchV. Eine Ansicht, die dies mit Verweis auf die Biogasdefinition des § 3 Nr. 10c EnWG für möglich erachtet, hat sich bislang nicht durchgesetzt.

[6] Nr. 9.3.2 sowie Nr. 9.3.1 Anhang 1 i.V.m. Nr. 17 Anhang 2 der 4 BImSchV.

[7] Mengenschwellen sieht auch der Störfallschutz nach der Störfall-Verordnung vor. Bei Wasserstoff gelten für den Anlagenbetreiber ab einer Menge von 5 t die Grundpflichten. Ab einer Menge von 50 t gelten zusätzliche Pflichten.

[8] §§ 30 ff BauGB.

[9] § 35 BauGB.

[10] Vgl. § 35 Abs. 1 und Abs. 2 BauGB.

[11] § 35 Abs. 1 Nr. 3 BauGB.

[12] BVerwG, BeckRS 2013, 54293.

[13] Zu beachten ist, dass das Erfordernis des direkten Grünstrombezugs durch Rentabiliätserwägungen im Sinne einer größtmöglichen Einsparung der Stromnebenkosten durch die Direktleitung nicht ausreichend zu begründen ist, um eine Ortsgebundenheit anzunehmen, vgl. Söfker, W. in: Ernst/Zinkahn/Bielenberger/Krautzberger, BauGB, § 35 Rn. 53.

[14] So jedenfalls Bringewat, J.: Rechtsfragen bei der Zulassung von Elektrolyseurprojekten, online abrufbar unter http://www.jurop.org/oeffbaurecht/aktuelle-rechtsfragen-bei-der-zulassung-von-elektrolyseurprojekten/ (zuletzt abgerufen am 12.12.2020).

[15] BVerwG, Urteil vom 22.01.2009, Az.: 4 C 17.07; Söfker, W.: in Ernst/Zinkahn/Bielenberg/Krautzberger, § 35 BauGB Rn. 34.

[16] § 34 BauGB.

[17] § 8 BauNVO, § 9 BauNVO.

[18] Schwab, R.: Auf dem Weg zu einer Wasserstoffinfrastruktur im Straßenverkehr, Berlin, 2006, S. 119.

[19] Henkel, J. in: Spannowsky/Hornmann/Kämper, BauNVO, § 14, Rn. 27.

[20] Henkel, J. in: Spannowsky/Hornmann/Kämper, BauNVO, § 14, Rn. 27.

[21] Vgl. BDEW, Strompreisbestandteile Juli 2020, online verfügbar unter: https://www.bdew.de/media/documents/201013_BDEW-Strompreisanalyse_Juli_2020-Haushalte_und_Industrie.pdf (zuletzt abgerufen am 09.12.2020).

[22] § 3 Nr. 25 EnWG bzw. § 3 Nr. 33 EEG 2021.

[23] Vgl. § 118 Abs. 6 S. 6 EnWG.

[24] Vgl. § 9a Abs. 1 Nr. 1 StromStG.

[25] Vgl. § 10 Abs. 1 StromStG. Bei einem Steuertarif von 20,50 € für 1 MWh (§ 3 StromStG) müsste ein Elektrolyseurbetreiber ca. 50 MWh Strom im Kalenderjahr steuerbelastet beziehen. Da der Strom an der Elektrolyse aber bereits befreit ist, müssten sich diese Stromsteuerkosten auf sonstigen Strom zu betrieblichen Zwecken beschränken. Ggf. bezieht eine Anlage auf der grünen Wiese solche Strommengen nicht.

[26] Vgl. § 9 Abs. 1 Nr. 3 lit. b) StromStG.

[27] Vgl. § 61 Abs. 1 EEG 2021.

[28] Vgl. §§ 63 ff. EEG 2021.

[29] Vgl. § 64 Abs. 1 Nr. 2 EEG 2021.

[30] § 64 Abs. 2 Nr. 1 EEG 2021, sog. Selbstbehalt.

[31] Vgl. § 64 Abs. 1 Nr. 1 i.V.m. Anhang 2 EEG 2021.

[32] Anhang 2 Nr. 77 EEG 2021.

[33] Vgl. § 64a Abs. 1 EEG 2021.

[34] Die Begrenzung greift auch für selbständige Teile eines Unternehmens, vgl. § 64a Abs. 5 EEG 2021.

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[36] Proost, J.: State-of-the art CAPEX data for water electrolysers, and their impact on renewable hydrogen price settings, International Journal of Hydrogen Energy, 2018, https://doi.org/10.1016/j.ijhydene.2018.07.164.

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[42] Agency for the Cooperation of Energy Regulators 2015, UIC Report – Electricity Infrastructure, Online verfügbar unter: http://www.acer.europa.eu/Official_documents/Acts_of_the_Agency/Publication/UIC%20Report%20%20-%20Electricity%20infrastructure.pdf

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[44] Agency for the Cooperation of Energy Regulators 2015, UIC Report – Electricity Infrastructure, online verfügbar unter: http://www.acer.europa.eu/Official_documents/Acts_of_the_Agency/Publication/UIC%20Report%20%20-%20Electricity%20infrastructure.pdf

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Contribution to Publications

	Chapter VI	**Chapter VII**	**Chapter VIII**	**Chapter IX**
Conceptualization	CS, JT	CS, TW	CS, KK, TS, PT, IN, AVG	CS, TW, TS
Methodology	CS, PT, AVG	CS, TW, DF	CS, KK, TS, PT, IN, AVG, SGR	CS, TW, TS
Validation	JT, AVG, SGR	CS, TW, DF	CS, IN, SGR	TW, TS
Formal Analysis	CS, JT, TW	CS, TW	CS, KK, IN	CS
Investigation	CS, JT, TW	CS, TW, DF	CS, KK, PT, IN, AVG, SGR	CS
Resources	CS, JT, TW	CS, TW	CS, KK, TS, PT, IN, AVG, SGR	CS, TW
Data curation	CS, JT, PT, TW	CS, TW, DF	CS	CS, TW
Writing	CS, JT, TW	CS, TW	CS, KK	CS
Editing	AVG, SGR, PT, JT, TW	EZ	TS, PT, IN, AVG, SGR	TW, TS
Visualization	CS	CS, TW, DF	CS, KK	CS
Supervision	CS, JT	CS, TW	IN, AVG, SGR	CS
Project Administration	CS, PT, JT, AVG	CS, TW, EZ	CS, PT, AVG	CS, TW
Funding Acquisition	AVG, SGR	CS, TW, EZ	CS, TS, AVG, SGR	CS, TW, TS

Abbreviations: CS: Christian Schnülle; JT: Jorg Thöming; PT: Pablo Thier; AVG: Arnim von Gleich; SGR: Stefan Gößling-Reisemann; TW: Timo Wassermann; DF: David Fuhrländer; EZ: Edwin Zondervan; IN: Igor Nikolic; KK: Kasper Kisjes.

Student Works Included in this Thesis

David Fuhrländer, Master thesis 2019, University of Bremen, *Analyse und Evaluation des modellierten Betriebsverhaltens von Elektrolyseuren bei fluktuierender Eingangsleistung*