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Energy System and Process Perspective on Sector-coupling Technologies – Influential Factors in Model-based Technology Benchmarks

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„Lorem ipsum dolor sit amet“

The comforting feeling when there are more than just blank pages at the start of a project.

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Abstract

The goal of climate protection by transforming energy systems into fully sustainable circular economies is no longer just part of the scientific discourse, but is increasingly being incorporated into law as a binding goal of our society. However, many open questions still need to be answered and discussed from different perspectives in order to make the necessary investments for a successful transformation. The diversity of stakeholders, the uncertainties in the development of individual technologies and non-technical boundary conditions are some of many challenges. Several approaches are currently being pursued in order to evaluate new technologies and to make investment decisions. The simulative approaches range from meta-studies, to models on the process level to high-resolution energy system models. The larger and more detailed the models become, the greater the need for abstraction and assumptions. However, this inevitably also induces a form of uncertainty in the results. Currently, these uncertainties or influencing factors are only discussed separately within the individual approach, for example at process level or at energy system level. This work aims to analyse all individual approaches separately using an example, an entrained flow gasification-based biomass-to-x plant, and in particular to work out the influencing factors. Subsequently, the individual results are to be placed in a broader context. It can be shown that the choice of feedstock in particular has a very large influence both at process level and at a systemic level, for example regarding the technology portfolio of a country. From the operator's point of view, the costs of the plant are of great importance, while the individual plant costs are of lesser importance from a system perspective and thus disregarding individual interests. Here, the influence of the costs is clearly outweighed by the demand patterns and the availability of the feedstock. For the future evaluation of new technologies in the context of sector coupling, it can be concluded that the sole consideration of the system level or the process level is not always sufficient. Rather, the methods should be further improved in order to be able to carry out holistic analyses in a more time-efficient manner. The application of such tools can then be used to provide more in-depth information for both political decision-makers and investments in the industry.

Kurzfassung

Klimaschutz wird aktuell vor allem durch die Transformation von Energiesystemen in vollständig nachhaltige Kreislaufwirtschaften vorangetrieben. Die Transformation selbst ist dabei nicht mehr nur Teil des wissenschaftlichen Diskurses, sondern wird zunehmend als verbindliches Ziel unserer Gesellschaft gesetzlich verankert. Allerdings sind noch viele offene Fragen zu klären und aus unterschiedlichen Perspektiven zu diskutieren, um die notwendigen Investitionen für eine erfolgreiche Transformation zu tätigen. Die Vielfalt der Akteure, die Unsicherheiten in der Entwicklung einzelner Technologien und nicht-technische Randbedingungen sind einige von vielen Herausforderungen. Derzeit werden verschiedene Ansätze verfolgt, um neue Technologien zu bewerten und Investitionsentscheidungen zu treffen. Die simulativen Ansätze reichen von Metastudien über Modelle auf Prozessebene bis hin zu hochauflösenden Energiesystemmodellen. Je größer und detaillierter die Modelle werden, desto größer ist der Bedarf an Abstraktion und Annahmen. Dies führt zwangsläufig auch zu einer Unsicherheit in den Ergebnissen. Derzeit werden diese Unsicherheiten und Einflussfaktoren nur innerhalb des einzelnen Ansatzes, zum Beispiel auf Prozessebene oder auf Energiesystemebene, separat diskutiert. Ziel dieser Arbeit ist es, am Beispiel einer Biomass-to-X Anlage auf Basis der Flugstromvergasung alle Einzelansätze separat zu analysieren und insbesondere die Einflussfaktoren herauszuarbeiten. Anschließend werden die Einzelergebnisse in einen breiteren Kontext gestellt. Es kann gezeigt werden, dass insbesondere die Wahl der Einsatzstoffe einen sehr großen Einfluss sowohl auf der Prozessebene als auch auf einer systemischen Ebene hat, zum Beispiel hinsichtlich des Technologieportfolios eines Landes. Aus Sicht des Betreibers sind die Kosten der Anlage von großer Bedeutung, während die Kosten der einzelnen Anlage aus einer Systemperspektive - und damit unter Vernachlässigung individueller Interessen - von geringerer Bedeutung sind. Hier überwiegt der Einfluss der Kosten deutlich gegenüber dem Nachfrageverhalten und der Verfügbarkeit der Einsatzstoffe. Für die zukünftige Bewertung neuer Technologien im Rahmen der Sektorkopplung lässt sich schlussfolgern, dass die alleinige Betrachtung der System- oder Prozessebene nicht immer ausreichend ist. Vielmehr sollten die Methoden weiter verbessert werden, um ganzheitliche Analysen zeiteffizienter durchführen zu können. Die Anwendung solcher Methoden kann dann dazu genutzt werden, sowohl für politische Entscheidungsträger als auch für Investitionen in der Industrie vertiefende Informationen zu liefern.

Contents

1 Introduction

Public discourse in society is no longer centred on the question of whether humans are contributing to climate change, but rather on the question of which path to a sustainable energy system should be taken. While progress in renewable electricity generation is promising, there are still several unanswered questions in the production of renewable heat and especially in the supply of sustainable energy carriers.

The respective shares of the currently used energy sources for mobility, industry, trade, commerce and services (TCS) and households are shown in Figure 1.1. With more than a quarter, the industry contributes with a non-neglectable share to the German energy demand. Within industrial applications, by far the largest share is currently provided by (fossil) energy carriers. While for some sectors, for example mobility, already promising purely electricity-based alternatives are available, individual applications, for example high-temperature heat supply, will always be based on energy carriers. Ueckerdt et al. categorise the applications into three groups: (1) direct electrification is possible and the most cost-effective option, (2) direct electrification is possible but more expensive than using sustainable energy carriers, and (3) applications that cannot be electrified [1]. Given that sustainable energy carriers are to be generated to a large extent using electricity-based processes, electricity from renewable energies will play a decisive role even in applications that are not directly electrified [2].

The greatest potential for renewables lies in the utilisation of wind and solar radiation [2]. In addition, geothermal energy and biomass will provide a considerable share, although this will be significantly lower due to the lower usable potential and competing, for example non-energy, applications. Due to the intermittent nature of wind and solar generation, renewable electricity generation is volatile and requires storage and flexible power plants to balance demand and supply. As power plants are not to be fuelled by fossil fuels in the future, only a limited set of technologies and fuels is available for power generation in times with reduced solar radiation and wind. The alternatives can be categorised into alternative fuels and storage technologies. While storage systems initially require an increase in production capacities in order to fill the storages, alternative fuels are flexible and can be used independently. The most basic sustainable feedstock is biomass. However, as biomass is only available to a limited extent, biogenic residues and waste are increasingly being discussed as an alternative feedstock.

In addition to the increasing demand for energy from renewable sources, industry and thus the

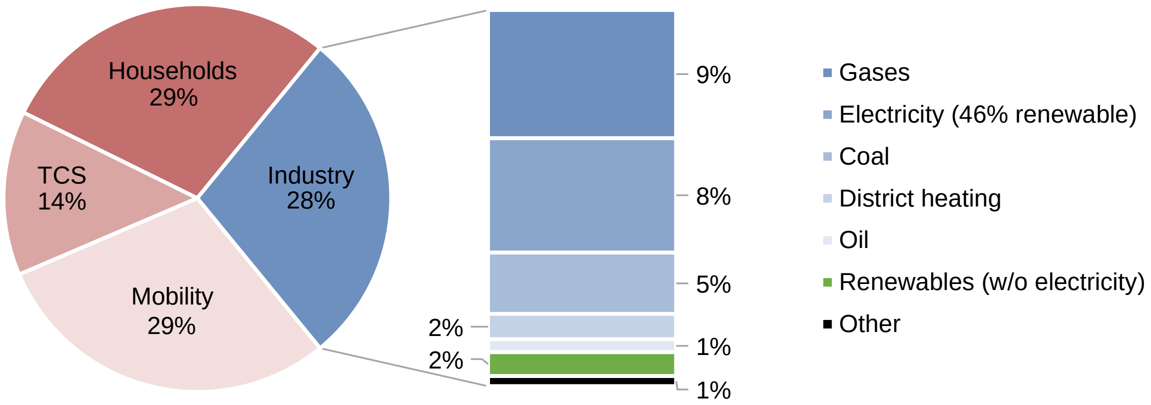

Figure 1.1: Overview of the relative energy consumption in Germany divided by sector (households, industry, mobility, and trade, commerce and services (TCS)), as well as the energy share in industry by energy carrier. Own illustration, data from [3].

production of goods must also be converted to renewable resources. Here too, fossil resources are currently the industry standard. If residual materials are not only used for energy supply, but also as feedstock for new products, this is referred to as a circular economy. Instead of a linear life cycle of products, the residual materials of goods are used as input materials for the production of new products after they have been used. The unavoidable losses within the circular process are to be compensated by renewable feedstock or electricity-based technologies. Here, too, biomass is to be recognised as a limited resource, thus making renewable electricity and techologies for recycling the driving forces behind the circular economy.

Various plant concepts are discussed that can enable a circular economy. One category of technologies are thermal processes that convert residual materials and waste into a gas suitable for use as a feedstock in industry. In particular, gasifiers are currently discussed, as they are already being operated on a large scale using fossil fuels. The use of entrained-flow gasifiers, for example, is already standard in many applications for the supply of liquid fuels or waxes from coal or gas.

Regardless of whether purely energetic or for the production of new raw materials, the use of alternative feedstocks leads to higher requirements for plants compared to their conventional fossil-fuelled counterparts. At the present time, investment decisions must already be made and the regulatory framework adapted in order to establish such new technology concepts on a long-term perspective. This raises the question how decision-makers in politics and companies can be supported by research. Resilient knowledge about the alternatives is required in order to choose a specific transformation path. This is where computer-aided methods come into play, which can generate an initial assessment of plant operation and possible applications even before demonstration plants are built. These models range from the process level, for example novel power-to-x systems, to cross-national system optimisation, for example modelling of a European hydrogen pipeline grid. The evaluation of an individual process or the comparison of several process variants usually starts at the process level, followed by cost estimates and a subsequent analysis of the possible applications on the overarching energy system level. However, these models are always an abstraction of reality and assumptions must be made. This means that the results of computer-aided analyses are always subject to uncertainty. The existing literature already discusses methods for taking uncertainties into account at the individual detail levels of modelling. However, there is a lack of standardised analyses that consider the entire process chain both from a process and system level, while discussing uncertainties.

A number of dissertations have already been written at the Chair of Energy Systems on the thematic focus of energy system analysis, concentrating on plant utilisation and the consideration of uncertainties. Buttler uses a simplified energy system model optimising the electricity sector to investigate the use of polygeneration plants for the production of electricity and methanol (MeOH) or synthetic natural gas (SNG) from coal [4]. The costs are compared with power-to-x systems. Miehling also uses an energy system model to optimise the design of power-to-methanol plants [5]. In both works, the focus is on the design of the plants and how these can be utilised most profitably from a system perspective. In contrast to Buttler and Miehling, Wedel does not use energy system optimisation to discuss specific plant designs and their use in future energy systems, but rather to analyse the uncertainties of individual system parameters on the optimisation results [6]. However, a joint consideration of (1) the plant-specific influencing factors on the efficiency and costs of the plant and (2) the energy system parameters that influence the result of the optimisation is still lacking. This approach requires both a techno-economic evaluation of the system at process level and sector-coupled modelling of the higher-level energy system with an evaluation of the influencing factors. If both analyses are available, combined broader implications can be drawn. This dissertation aims to combine both a detailed process level approach and a system perspective.

1.1 Outline

This publication-based dissertation consists of six publications, which are referred to in the text as **Articles I** to **VI**. A list of all publications is given in section 1.2, with all articles attached in full-text in Appendix A. Figure 1.2 gives an overview of the thesis structure in terms of both publications and content.

After the introduction, chapter 2 provides an overview of the fundamentals of alternative processes for sustainable energy carrier production from non-fossil sources, as well as current topics in energy system analysis. In this context **Article I** deals in section 2.2 with a meta-analysis of system studies on the demand for large-scale power plants in the energy transition. Furthermore, a differentiation from existing dissertations can be found in the fundamentals in chapter 2. Summarising the current state of literature and available methods, chapter 3 formulates the research question to be addressed. In a next step, chapter 4 introduces the methods used for process simulation, techno-economic assessment, and energy system modelling. **Article II** presents in section 4.5 the framework of an energy system model.

The results of the work are presented in chapter 5, focusing on the process level, and chapter 6, evaluating the systems level. Therefore, chapter 5 is divided into **Article III** (5.1), focusing on technical and energetic parameters of biomass-to-x plants based on biogenic residues, and **Article IV** (5.2), evaluating economic indicators. In chapter 6 the analysis focuses on the system perspective. Here, **Article V** (6.1) focuses on the general impact of foresight horizons, followed by **Article VI** (6.2), analysing influential factors on system optimisation models in general.

The results of each chapter and article are contextualised and discussed in chapter 7, including potential limitations within the study.

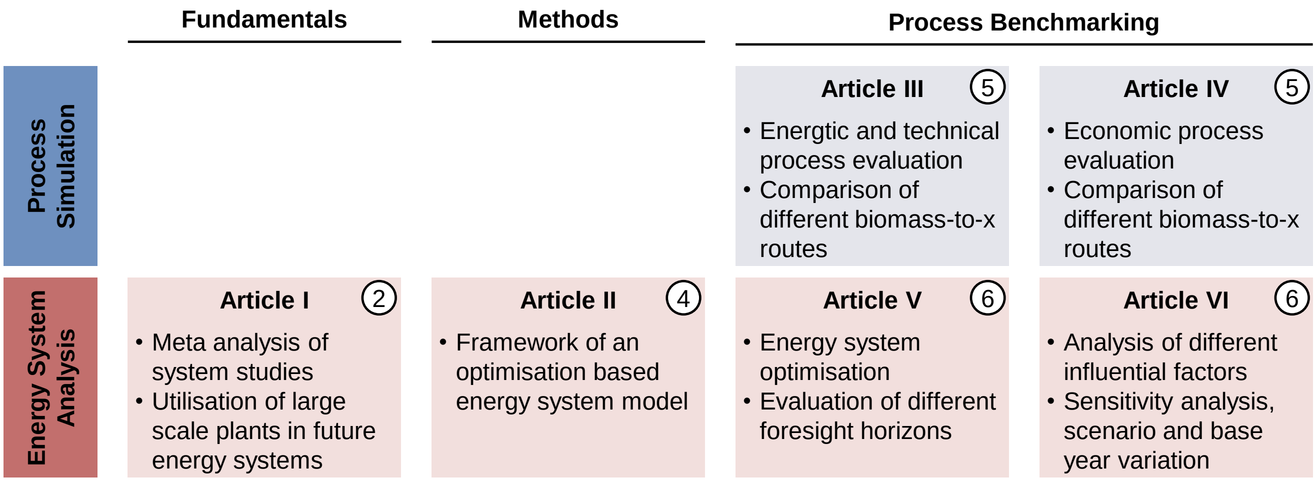

Figure 1.2: Allocation of Articles I to VI in the structure of the dissertation. The chapters are indicated within the circles.

1.2 List of Publications

All publications included in the dissertation are listed below. The articles themselves are appended in Appendix A. In addition, summaries of the articles and the respective contributions of the co-authors are provided in the respective thematic sections.

Article I:
Andreas Hanel, Sebastian Fendt, Hartmut Spliethoff (2022): *Operation of Conventional Power Plants During the German Energy Transition: a Mini Review*. In: Front. Energy Res. doi:10.3389/fenrg.2022.907251
Summary in section 2.2 and full-length article in section A.1.

Article II:
Sebastian Miehling†, **Andreas Hanel**†, Jerry Lambert, Sebastian Fendt, Hartmut Spliethoff (2023): *Energy System Optimization using (Mixed Integer) Linear Programming*. In: arXiv. doi:10.48550/arXiv.2308.01882
Summary in section 4.5 and full-length article in section A.2.

Article III:
Andreas Hanel, Vincent Dieterich, Sebastian Bastek, Hartmut Spliethoff, Sebastian Fendt (2022): *Entrained flow gasification-based biomass-to-X processes: An energetic and technical evaluation*. In: Energy Convers. Manag. doi:10.1016/j.enconman.2022.116424
Summary in section 5.1 and full-length article in section A.3.

Article IV:
Vincent Dieterich, **Andreas Hanel**, Sebastian Bastek, Hartmut Spliethoff, Sebastian Fendt (2024): *Entrained flow gasification-based biomass-to-X processes: A techno-economic assessment*. In: Energy Convers. Manag. doi:10.1016/j.enconman.2024.118061
Summary in section 5.2 and full-length article in section A.4.

Article V:
Jerry Lambert†, **Andreas Hanel**†, Sebastian Fendt, Hartmut Spliethoff (2023): *Evaluation of sector-coupled energy systems using different foresight horizons*. In: Renew. Sust. Energ. Rev. doi:10.1016/j.rser.2023.113562
Summary in section 6.1 and full-length article in section A.5.

Article VI:
Andreas Hanel, Toni Seibold, Johanna Gebhard, Sebastian Fendt, Hartmut Spliethoff (2024): *Evaluation of influential factors on energy system optimisation*. In: Energy Convers. Manag. doi:10.1016/j.enconman.2024.119156
Summary in section 6.2 and full-length article in section A.6.

† Dual-first authorship.

2 Fundamentals

This chapter provides a general introduction to energy systems and energy system analysis (section 2.1), including a summary of the current development of the German energy system. In particular, a meta-analysis of current system studies is presented in section 2.2 (**Article I**). Building on a definition and background knowledge on sector coupling (section 2.3), fundamentals on biomass- and waste-to-x (section 2.4), power-to-x (section 2.5) and synthesis of synthetic energy carriers (section 2.6) are presented.

2.1 Fundamentals of Energy Systems

In general, an energy system is understood to be the "entirety of systems and facilities for the generation, conversion, storage and distribution of various types of energy" [7]. Therefore, this includes the areas of electricity, heat, freight and passenger transport, as well as the supply of raw materials for industry. The science that deals with the development and evaluation of energy systems is referred to as energy system analysis. This section summarises the basics of energy systems and the German energy system in particular, which is later used as an example for case studies. Furthermore, common energy system analysis approaches are discussed and the consideration of uncertainties is addressed.

2.1.1 Germany Energy System

There are two ways of describing an energy system: Firstly, which energy demands are requested and secondly, which energy carriers and technologies are used to meet the demands. As shown in Figure 1.1, energy demand in Germany is divided into four sectors: households, mobility/transport, industry and TCS [3]. Each sector has characteristic demand structures in terms of the energy type. Figure 2.1-a summarises the primary energy demand in Germany, which adds up to around 3,000 TWh in 2023 [8]. This shows that Germany is still more than 75 % dependent on fossil energy carriers. While around half of electricity generation in the same year (Figure 2.1-b) is covered by renewable energies, dependence on fossil fuels such as mineral oil and natural gas remains high, primarily due to demand in transportation and industry [9].

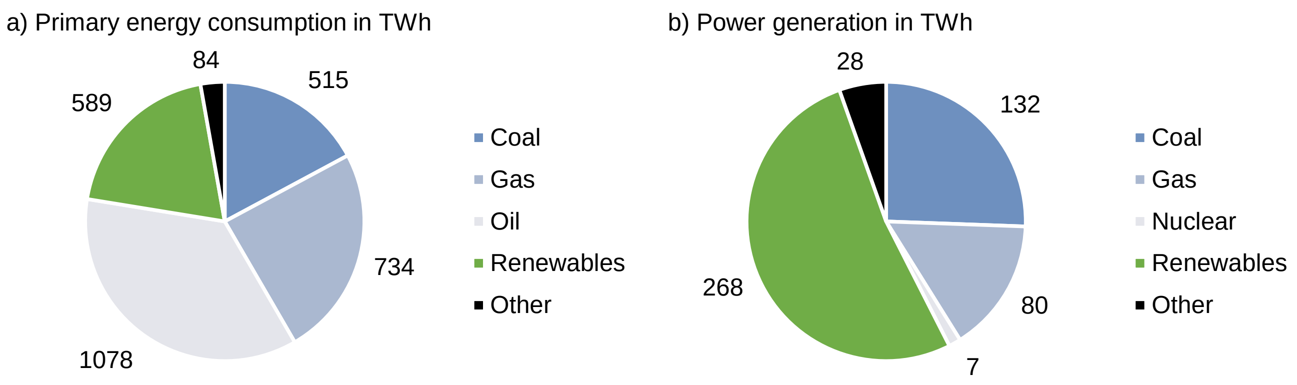

Figure 2.1: Primary energy demand (a) and power generation (b) in Germany 2023. Own illustration, data from [8, 9].

The aim of reducing the use of fossil fuels is based on the environmentally harmful effect of the emissions associated with their use and the limited availability of these resources. The emission of carbon dioxide (CO_2), or the emission of climate-impacting gases, is widely used as an indicator of the environmental compatibility of systems. Figure 2.2 shows the historical development of CO_2 emissions and Germany's emission targets up to 2045. In order to achieve net-zero emissions by 2045, all fossil applications must therefore be replaced by renewable technologies. This includes, among other things, the supply of electricity from renewable energies through wind turbines and solar power systems. Figure 2.2 shows the expansion of wind and solar utilisation to date and the ambitious targets for installed capacity by 2040.

As renewable electricity is the simplest and most efficient way of providing sustainable energy, the electrification of fossil fuelled processes is the primary objective [2]. Individual transport in particular, as well as some heating and industrial applications, have already been recognised as areas that are easy to transform. However, as shown in [1], electrification is not necessarily the most cost-effective transformation pathway in, for example, freight transport, the steel industry or cement production. Furthermore, there are applications that cannot be electrified. The promotion of a hydrogen (H_2) economy and thus H_2 as the energy carrier to replace natural gas in the future, is intended to enable the import of energy over longer distances, delayed utilisation and broader applicability than with electricity alone.

Expectations for the future energy supply assume that electricity generation will stabilise at over 1,000 TWh [2], compared to 515 TWh today as shown in Figure 2.1-b), and H_2 demand will also reach 1,000 TWh [10]. Although the aim is to cover the electricity demand with national electricity generation, it will not be sufficient to cover the H_2 demand via water electrolysis and, thus, the major amount of synthetic energy carriers like H_2 will be imported.

On the technology side, it is assumed that the vast majority of electricity requirements will be covered by wind turbines and photovoltaics. On the energy carrier side, however, the decision beyond H_2 has not yet been made, as the industry is also dependent on carbon as a reactant for its products. One reason is the entry stage of the development of promising technologies to cover long-term and large-scale investments. Regardless of the chosen technology, the first step here is the introduction of a circular economy, keeping carbon in the cycle through material and chemical recycling. This reduces the demand for carbon and, depending on the chosen type of imported

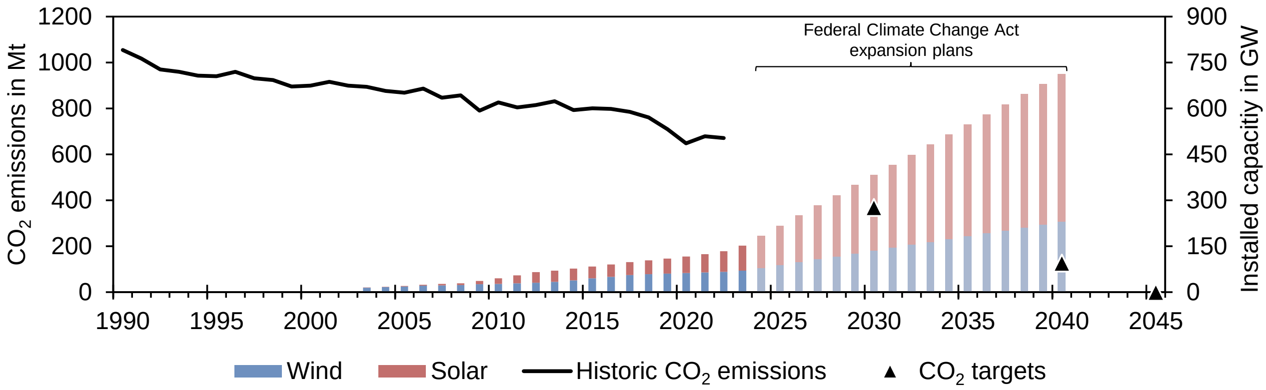

Figure 2.2: Historic data and targets for CO_2 emissions and renewable technology capacities in Germany. Own illustration, data from [11–13] and §§3-4 Federal Climate Change Act 2023 (EEG 2023).

energy carrier, H_2 import. Consequently, this is associated with a reduction in the demand for national electricity generation.

The future development of energy systems is analysed in energy system studies, which in general are discussed in more detail in subsection 2.1.2. However, as a large number of studies have already been published on Germany, **Article I** (section 2.2) takes a detailed look at the development of the power plant portfolio in Germany during the energy transition in the form of a meta-study.

In addition to national challenges, the boundary conditions existing due to the strong interconnection within Europe must always be taken into account. For example, the electricity supply is based on an interconnected European grid. Similarly, a Europe-wide H_2 network is planned, analogous to today's gas network.

Overall, there is still some uncertainty about how energy systems, such as the German energy system, should develop in order to achieve the climate targets and at the same time maintain the economic and social standard of living. Since, unlike individual technologies, no prototypes can be used for testing entire energy systems, decisions can only be made on the basis of model calculations. Energy system modelling used and their analyses have grown into a whole field of research.

2.1.2 Energy System Analysis

The field of energy system analysis is very broad and incorporates all issues related to the shaping of a region's current and future energy supply. Thematically, it includes technical, social, political and economic matters. However, the common denominator is usually the question of how a sustainable energy supply can be ensured in the long term [14]. This thesis focuses in particular on technical and economic issues, specifically in the field of energy system studies. These are increasingly being used in political and social discussions, as well as for investment decisions [2]. Due to the increasing complexity of the models on which the studies are based, more and more attention is being drawn to the uncertainties in the study results. This section is intended to provide the necessary knowledge about energy system studies and their current applications, whereas ways of discussing uncertainties are presented in subsection 2.1.3.

History of Energy System Analysis

In an extensive review of research on 100 % renewable energy systems, published by Breyer et al., key milestones in the field are presented. They identify that the first 100 % renewable energy system study was published as early as 1975. While initially only a few articles were published each year, the field of research began to grow rapidly from the 2000s onwards. The first modelling frameworks were also published at this time and some of them were made freely available as open source software. Even if individual regions are still much more strongly represented today, mainly due to their research history, and thus more studies have been published on their regions, there are now energy system studies on 100 % renewable energy supply for almost every major economy. [15]

In addition to the increasing growth within the 100 % renewable systems, criticism of the feasibility of such systems is also increasing. The main points criticised are (1) return on investment, (2) volatility and stability, (3) cost assumptions, (4) raw material demand and (5) social resistance and energy injustice. However, according to Breyer et al., independent research groups have been able to identify several feasible routes to a 100 % renewable energy supply, despite initial criticism. [15]

Even though the energy system analysis is already well advanced, there are still a number of unresolved issues from today's perspective. For example, most studies do not take industry into account, or do so only partially or in a highly abstracted manner. However, as industry is one of the most difficult sectors to transform, a special focus should be placed on modelling the transformation of industry. The high demand for raw materials used in the construction of renewable energy technologies is also criticised. Today, only an established circular economy is seen as a possible model for operating a functioning 100 % sustainable energy system with the available raw materials. In addition to analysing the energy system, the process development of technologies is particularly important here. In addition to the raw materials for technologies, the availability of renewables itself is also a factor with significant uncertainty, as, for example, the availability of water for hydropower plants or the growth of biomass can be strongly influenced by climate change. Just like the availability itself, the volatility of solar irradiation and wind will also increasingly influence the system as the share of renewables grows. The stability of electricity grids in particular must be rethought as they will change from the current concept based on a few large-scale power plants to a high number of volatile small suppliers. While topics relating to the electricity grid and its stability have already been analysed many times, the use of heating and cooling grids has only been a marginal topic to date. However, existing studies show that the utilisation of grid-connected heating/cooling in particular can provide an enormous systemic advantage. One of the reasons for this is the possibility of integrating waste heat and utilising geothermal energy. In addition to the technical issues, the influence of society is also increasingly being analysed, as well as the influence of global energy trade with the global south and the associated energy injustice. [15]

Nonetheless, as stated by Lund et al., "the main purpose of energy systems modelling is to assist in the design, planning and implementation of future energy systems" [14]. This goal should not be neglected while, most likely iteratively, all the open points are cumulatively integrated into the energy system analysis.

Approaches in Energy System Analysis

Considering the selected example of Germany, most of the existing literature on energy system analysis is based on the optimisation of energy systems. In most cases, a small number of scenarios are compared with a reference scenario and recommendations for action are derived from the differences in the results. The definition or categorisation of the scenarios into typical categories allows for four or five groups. The following list is taken directly from: [16]

- "**Trend:** Trend scenarios are based on the extrapolation of current political and legal measures into the future. Therefore, no additional expansion targets or other further constraints are imposed on the model.
- **Reference:** The term reference scenario is generally used to describe scenarios that are used as the basis of a more advanced comparison. Moderate developments are often assumed for the future, which means that trend scenarios are usually used as a reference.
- **Ambitious:** Ambitious scenarios refer to scenarios that go beyond current policies. In most cases, this means a faster or stronger reduction of greenhouse gas emissions or an accelerated expansion of renewable energies. However, this can also mean societal aspects, such as a change in values toward energy saving behaviors.
- **Low ambition:** Low-ambition scenarios represent the opposite compared to the ambitious ones. Climate protection targets are given low priority overall. For example, existing climate protection measures are dropped or missed. Also considered here is possible societal unacceptance toward savings measures or individual technologies.
- **Other:** If a scenario cannot be assigned to any of the four categories mentioned, it is classified as another scenario."

In contrast, less attention is paid to analysing the influence of changing base years and changing foresight horizons. Detailed sensitivity analyses are also rare. Although these three influencing parameters are already discussed in individual studies and in some cases already attached to scenario-based studies, a combined analysis in which the respective influence compared to each other is lacking [17]. However, what all studies and analyses have in common is that energy systems are becoming increasingly complex and the various supply and demand structures are being linked with each other via so-called sector coupling. Sector coupling usually also refers to the technological possibilities of coupling several forms of energy in order to achieve flexibility in the system. A detailed definition and a description of the technologies involved can be found in sections 2.3-2.6.

2.1.3 Sensitivity and Uncertainty

The wide range of applicability of energy system models and the large number of parameters required already indicate that energy system analysis is becoming significantly more complex. As complexity increases, the necessity for accurate interpretation and discussion of the results also increases, as the results are only valid for the specific case modelled. Consequently, there has been a growing trend in the development and utilisation of methods that evaluate the sensitivity of energy system models or deliberately project uncertainties from assumptions onto the results.

Yue et al. categorises the available methods in uncertainty consideration into four groups: Monte Carlo simulations, stochastic programming, robust optimisation and modelling to generate alternatives [18]. A common feature of these methods is that they either allow uncertainty to be quantified or identify the most robust solution within the solution space. However, it is not possible to draw conclusions about the input parameters that influence the uncertainty the most. A further challenge in the quantification of uncertainties is the need for a large number of simulations, whereby the use of artificial neural networks, for example, attempts to reduce the computational effort [19]. Additionally, the required probability density function per input parameter can limit the applicability of the method. Due to the large number of individual applications and methodological approaches, detailed descriptions and examples can be found in the existing literature, such as the review by Feng et al. [20].

In contrast to the quantification of uncertainties, sensitivity analysis is used to identify a correlation between input parameters and the simulation results. Those correlations can be used for both the individual significance of an input as well as the interactions between various input parameters [21]. One possibility here is the step-by-step change of individual input parameters, also known as "one-factor-at-a-time", which according to Saltelli et al. only leads to valid results for linear models [22]. Campolongo et al. further distinguish between global and local methods, as well as a quantification of the individual parameter influences or simply a qualitative ranking [23]. In this context, global is referred to as the consideration of the the entire real existing value space of an input parameter instead of just a (local) variation around the base case value. In the case of global sensitivity analysis, Usher et al. list three possible approaches [21]: variance-based, method of Morris and meta modelling. The Morris method is particularly suitable for application to energy system models, as the variance-based approach with $500(k+2)^*$ simulations requires a significant amount of computing time and meta-modelling requires known realisations or simplifications within the model [21]. Summarised, depending on the chosen input space, the Morris method can be described as global, qualitative sensitivity analysis [23]. If a quantification is needed, methods like Sobol or FAST can be used.

In this work, the so-called Morris method is used, which was introduced by Morris using *elementary effects (EE)* as indicators [24]. Radaideh et al. summarise several methods and, for example, describe in detail the application of the Morris method on energy system models [25]. The calculation of the *EE* is defined as in Equation 2.1 by the ratio of the difference between the results of two simulations f(x) and the difference between the respective varied input parameters:

$$EE_i^{(r)} = \frac{f(x_i^{(r)}) - f(x_{i-1}^{(r)})}{\Delta_i} \text{ with } i \in N_{Parameters}, r \in R_{Permutations} \tag{2.1}$$

According to Campolongo et al., between five and fifteen variations per input parameter are carried out for the Morris method [23]. In order to fill the parameter space as optimally as possible, the use of Latin hypercube sampling is suggested [24].

Finally, the mean value, absolute mean value and variance are used to qualitatively interpret the respective EEs. According to Radaideh et al. the effect of an input parameter is significant, if the absolute mean value is high [25]. Additionally, a high variance in the EE can be interpreted with a high interaction between the respective input parameter and other input parameters.

* k corresponds to the number of input parameters

2.2 Operation of Conventional Power Plants During the German Energy Transition: A Mini Review (Article I)

The following section serves as a summary of the results of the in section A.1 attached article. The contents of this section were published in:

Andreas Hanel, Sebastian Fendt, Hartmut Spliethoff (2022): Operation of Conventional Power Plants During the German Energy Transition: a Mini Review. In: Front. Energy Res. doi:10.3389/fenrg.2022.907251.

Summary In this article, a meta-analysis of existing energy system studies on the transformation of the German energy system is performed. It focuses on the expected demand for conventional power plant capacity and the use of conventional power plants as a bridging technology during the energy transition. By definition, meta-studies consist exclusively of contents of the used primary sources, in this case, the system studies. Thus, the authors calculate no new scenario analyses and all results are extracted from previously selected studies. A prerequisite for the selection of a study is a scope up to at least 2030, in the best case up to 2050. Only studies are included that were published from 2017 onwards and thematically address the quantitative development of the electricity sector in Germany. Based on these specifications, the data basis of the evaluation is composed of 38 system studies, most of which are using optimization models to analyse the energy system. While the clients range from purely scientific institutes to political associations and interest groups, the authors of most of the studies are scientific institutions or consulting firms.

Technologically, the analysis is focused on gas-fired power plants, as both coal and nuclear power plants will phase out due to political decisions. Altogether, conventional power plants covered 50 % of the net power generation in Germany in 2021. Summarizing the historical development of natural gas utilization in power plants, besides a drop during the mid-2010s, the level has had an increasing trend during the last 30 years. This drop in the net power generation during a period of constant electricity demand results from high natural gas prices and simultaneously low CO_2 emission allowance prices. The increase in gas-fired power plant use in terms of net electricity generation in the years to 2020 is significantly underestimated in most system studies. The median of the studies at 70 TWh is well below the actual 95 TWh provided.

The peak of natural gas utilisation is expected by most of the studies between 2030 and 2040, with a maximum of about 100 TWh of net power generation. Besides one scenario, natural gas power plants at least are operated until 2040. By separating trend and “business as usual” scenarios from more ambitious scenarios, the trend towards longer usage of natural gas can be seen in the first group. By considering both, natural gas and synthetic natural gas, the calculated peak of power plant utilisation shifts slightly towards 2040. Additionally, the demand for conventional power plants extends further until 2050 and beyond. Therefore, the demand for synthetic energy carriers can be expected to rise from 2040. As those energy carriers are assumed to be climate neutral, power plants which are constructed in the late 2030s are used to provide flexibility in future energy systems. The demand for synthetic energy carriers will mostly be driven by demands for heat, transportation and chemicals. Overall, if the median of all studies is considered, an increase from 2.5 GW of installed power-to-gas applications in 2030 to 40 GW in 2040 is expected. This, however,

is likely to not cover the rising demand for power-to-x products. Therefore, an additional import of power-to-x products in 2050 of more than 350 TWh is predicted.

Nowadays, gas-fired power plants in Germany are operated on average with $3000\,h\,a^{-1}$, the studies median expects a decrease to around $1230\,h\,a^{-1}$ in 2050. This shows, that the conventional centralised power plants will mostly be used to provide flexibility. The results of the analysed energy system studies depend on various boundary conditions. Additionally to the before mentioned scenario types (trend vs. ambitious), for example, the technological openness, which is defined as the number of degrees of freedom in the choice of technologies, of the model has a strong impact on the systems development. The installed capacities peak in more open scenarios is expected to be at 53 GW, whereas the more restricted scenarios only expect 39 GW of maximum installed capacities.

In summary, the meta-analysis shows that conventional power plants or systems with comparable characteristics will be particularly important for the transformation of the energy system towards a 100 % sustainable system. There will be a feedstock shift from natural gas to synthetic fuels, as well as a reduction in full load hours. However, further studies with much more flexible models are needed to evaluate the actual flexibility needs and the interaction with sector-coupling technologies.

Contributions This paper is the result of the common effort of more authors. **Andreas Hanel:** Writing original draft, data analysis and concept development, **Sebastian Fendt:** Concept development and supervision, **Hartmut Spliethoff:** Concept development and supervision. All authors reviewed the manuscript.

2.3 Sector Coupling

The concept of sector coupling (subsection 2.3.1) and the range of technologies to be considered here (subsection 2.3.2) will be motivated in the following sections.

2.3.1 Interpretation of Sector Coupling

As shown in **Article I**, sector coupling and the use of new technologies are becoming increasingly important. Based on the present analysis, the direct use of fossil fuels will be replaced in the medium term by synthetic energy carriers, which will act as a substitute and especially as a long-term storage possibility. However, the term sector coupling not only covers the intermediate storage of renewable electricity in energy carriers for later reconversion into electricity, but according to Ramsebner et al., includes all consumer groups and forms of energy on the demand side [26]. As shown in Figure 2.3, not all energy sources are allocated to all consumer groups. While electricity is used in all sectors, only industry is dependent on electricity, (process) heat and energy carriers of various different forms.

Categorisation of energy sectors	Consumer group			
	Industry	Transport	Residential	TCS
Energy: Electricity	●	●	●	●
Energy: Heat	●		●	●
Energy: Fuels and chemicals	●	●		○

Figure 2.3: Overview of different energy demands of the sectors industry, transportation, residential, and trade, commerce and services (TCS).

The aim is always to keep the costs of the entire system as low as possible and to maximise profits. Additionally, the overarching boundary condition of reducing greenhouse gas emissions must be considered. If the goal of reducing emissions is strictly defined, the most favourable technologies are used first. As shown in [1], the specific CO_2 avoidance costs increase depending on the application. Initially, the use of direct electrification is easy and relatively cheap to implement in some cases, such as private and passenger transport, space heating and domestic hot water, as well as TCS. In further areas of application, such as high-temperature systems, freight transport or the steel and cement industry, electrification is technologically possible but not necessarily cheaper and more efficient than the use of synthetic energy carriers. When it comes to the supply of chemicals as well as air and sea transport, only synthetic energy carriers will be used. Finally, there are also applications that have process-related emissions and will therefore be dependent on measures such as CO_2 capture or emission compensation products.

For easier understanding, it is important to distinguish between the demand side and the supply side when describing sector coupling. In both cases, the underlying question usually relates to flexibilisation of the energy system in order to balance out the volatile supply of renewable electricity from solar radiation and wind. While volatility on the supply side can be utilised profitably through flexible technologies, flexibility in demand is not always possible or desired on the consumer side. In this context, self-generation and self-consumption optimisation must also be taken into account.

In this work, the analysis of sector coupling is defined so that all demand groups (see consumer groups in Figure 2.3) with their respective specific energy requirements are taken into account and the supply side is optimised accordingly. In addition to electricity and heat, in particular several synthetic energy carriers play a role as a cross-sector exchange in order to evaluate flexibility and storage measures.

There are already a large number of technologies that are categorised according its ability to supply flexibility, for example via sector coupling. Just as many studies on their potential applications have already been published and discussed in the scientific community. Nevertheless, it has not yet been conclusively clarified, which technology will be used for which purpose, particularly due to current uncertainties regarding further technological developments. In summary, the uncertainties within the studies have not yet been sufficiently considered and analysed.

2.3.2 Technologies for Sector Coupling and Flexibilty

Energy system analysis is used as a tool to study the interaction of all these technologies and in particular to identify the most favourable technology portfolios from a system perspective (see section 2.1). The incorporated technologies can be divided into the following groups:

- **Storage systems:**
  To store energy, systems for electricity (for example battery storage, pumped hydro storage), heat (for example latent water storage, phase change material storage) and energy carriers (for example caverns, tanks) are analysed.
- **Demand side management:**
  In demand side management, consumers, both private and industrial, are ramped up and down in a system-orientated manner in order to smooth the demand curve.
- **Polygeneration:**
  In contrast to conventional single-generation plants, polygeneration plants produce two or more products, ideally in a flexible ratio.
- **Heat integration:**
  Both the energetic optimisation of processes via heat integration and the coupling of waste heat into heating networks serve to increase flexibility and efficiency.
- **Biomass- and waste-to-x:**
  Discussed in detail in section 2.4.
- **Power-to-x:**
  Discussed in detail in section 2.5.
- **Synthetic energy carrier:**
  Discussed in detail in section 2.6.

2.4 Biomass- and Waste-to-X

With the exception of heat generation from biomass, the utilisation of solid fuels has long involved mainly lignite and hard coal, as well as the disposal of waste. With the transition of the energy sector and industry away from fossil fuels, the focus is increasingly shifting to biomass, biogenic residues and waste. As shown in Figure 2.4, two basic processes can be distinguished:

- Combustion: full oxidation of the feedstock, mainly for power and heat supply
- Gasification: partial oxidation of the feedstock, mainly for synthesis gas production

Given the assumption that electricity in future energy systems will mainly be provided by photovoltaics and wind power and that heat, with the exception of high-temperature applications, will mostly be provided by electricity, the focus in the utilisation of limited sustainable solid feedstock will be on the synthesis of energy carriers and thus on synthesis gas production. Even if synthesis gas can also be used for power generation, for example in gas turbines, fuel cells or gas engines, and heat generation, for example in gas boilers, those processes are not considered as main application. However, as flexibility in energy systems are becoming more relevant, co- or polygeneration of more than one single product can be of interest. Despite the possibility of being able to provide a feedstock for syntheses by CO_2 sequestration, this process route is not considered further.

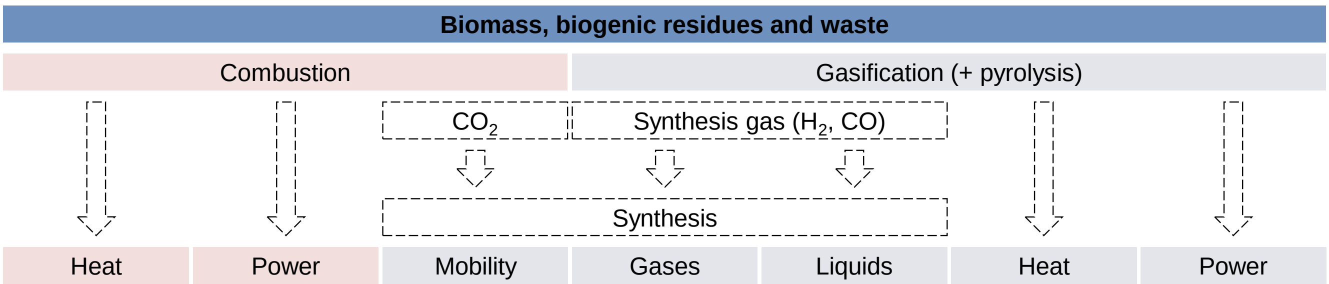

Figure 2.4: Schematic illustration of the potential thermochemical ways of utilising biomass, biogenic residues and waste for various applications.

2.4.1 Synthesis Gas from Biomass and Waste

The supply of synthesis gas can be divided into the technical steps of feedstock pretreatment, gasification and synthesis gas conditioning. In order to motivate the need for pretreatment and conditioning of the raw gas, gasification is discussed first.

Gasification The gasification of (solid) feedstocks is a state-of-the-art thermochemical process. The aim of gasification is the almost complete conversion of the feedstock into a synthesis gas that is available as a secondary energy source for further applications. In principle, the gasification process can be divided into three intermediate steps: heating, release of volatiles and gasification, which in idealised terms take place one after the other. The process of releasing volatiles in an inert environment is referred to as pyrolysis. This thermochemical process produces gaseous but, cooled to ambient conditions, also liquid and solid products. The thermal processing of feedstocks is summarised in simplified form in Figure 2.5. [27]

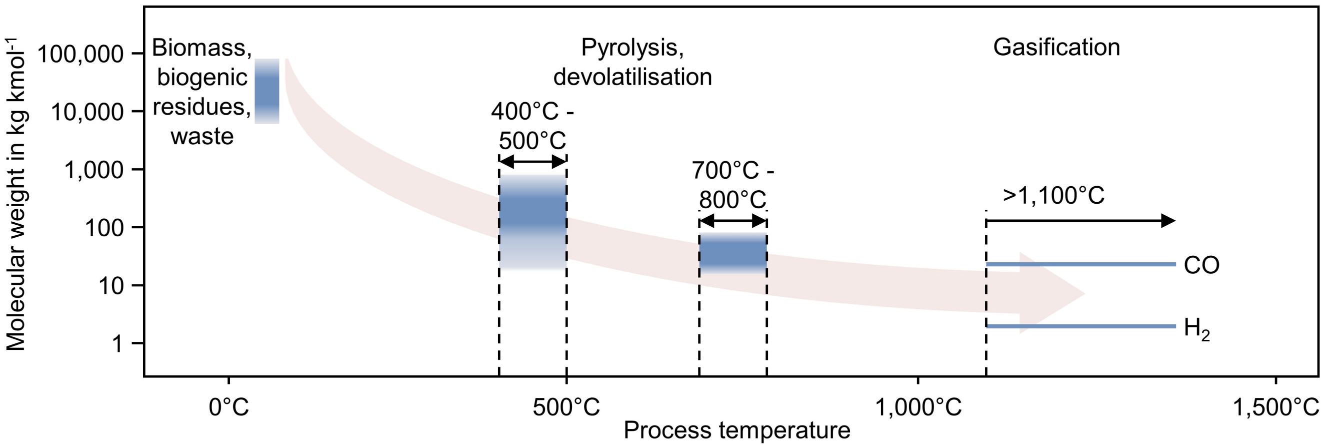

Figure 2.5: Simplified illustration of the dependence of products on temperature in the thermal conversion of biomass, biogenic residues and waste. Own illustration based on [28].

Upon entering the gasification zone, the feedstock is rapidly heated, which leads to the drying and subsequent release of the water it contains without changing its chemical composition. Devolatilisation (or pyrolysis) begins at temperatures of around 350 °C and marks the start at which the complex macromolecular arrangement of the feedstock, for example biomass with cellulose, hemicellulose and lignin, is transformed into solid coke alongside various gaseous by-products. The actual gasification process begins at around 800 °C and leads to a reaction between coke, gases and the gasification medium to form H_2 and carbon monoxide (CO). Besides the combustion reactions of C, CO, H_2 and methane (CH_4), gasification can be described by the following equilibrium reactions: [27]

- Boudouard reaction: $C + CO_2 \rightleftharpoons 2\,CO$
- Water gas reaction: $C + H_2O \rightleftharpoons CO + H_2$
- Methanation reaction: $C + 2\,H_2 \rightleftharpoons CH_4$
- Methane reforming reaction: $CH_4 + H_2O \rightleftharpoons CO + 3\,H_2$
- CO shift reaction: $CO + H_2O \rightleftharpoons CO_2 + H_2$

Overall, gasification is an endothermic process and therefore requires an energy supply, for example provided by the combustion reactions in conventional process concepts. Besides utilising part of the feedstock, external energy sources can also be used, such as external heating of the reaction chamber or plasma integration into the reaction zone. Here, the motivation is always to increase the conversion, for example the carbon content in the synthesis gas (in the form of CO). Depending on the desired product gas, the gasification medium is selected. In principle, air, oxygen, CO_2 or steam are possible options. Compared to pure oxygen, air has the disadvantage of carrying inert nitrogen into the reactor, which then remains in the raw gas for downstream applications. Selecting steam or CO_2 as the (co-)gasification medium allows the H_2/CO ratio in the product gas to be adjusted. [27]

The technical realisation of gasification an be divided into three reactor concepts: Fixed bed gasification, fluidised bed gasification and entrained flow gasification. *Fixed-bed gasifiers* are characterised by having a solid feedstock that is not transported by the gasification medium or raw gas. A solid bed moves against or with the gasification reaction zone, driven by gravity. However, the comparatively simple design is accompanied by increased proportions of pyrolysis product in the raw gas. *Fluidised bed* gasification is characterised by fluidisation of the feedstock by the gasification medium, which significantly improves both energy and mass transfer. Most of the material in the reactor is inert (for example ash or sand) and remains in the reactor while the raw gas leaves the reactor. Compared to the fixed bed, the conversion is higher. However, the gasification temperature is limited by the ash melting point of the feedstock, as melting can lead to agglomerates in the fluidised bed, which can impair the process to the point of stopping it. The particle size is also limited, as material that is too fine is carried out of the fluidised bed and large material will not be fluidised. In *entrained-flow gasification*, the feedstock is finely ground ($<200\,\mu$m) and blown into the reactor together with the gasification medium. The process is operated at higher temperatures than the other reactor concepts in order to guarantee complete conversion with a short residence time. Due to the high temperatures of well above 1100 °C, a particularly high product gas quality can be achieved. The need for finely ground feedstock means that pretreatment is necessary, especially for alternative feedstocks. [27]

Although the use of alternative raw materials such as biomass, biogenic residues and waste for gasification still requires further research, it is mentioned and investigated as a core component in many research projects and plant concepts. In particular, entrained-flow gasification is characterised by several advantages, as summarised in: [29]

- "Deployable for large scale plants
- Almost complete tar conversion
- Mature technology (used in large scale for coal-to-liquid)
- Pressurized operation possible
- Cold gas efficiency up to 90 %
- Expected direct power integration, e.g. plasma torch"

Pretreatment In contrast to fossil feedstocks, for example coal, the characteristics such as elemental composition and physical properties of alternative feedstocks are much more widely dispersed. In raw form, the energy density is usually lower, the feedstock is more heterogeneous and often contains more unwanted or even harmful components [30]. For this reason, extended pretreatment is often necessary in addition to drying and grinding. Two main technological approaches can be found in the literature: hydrothermal carbonisation and torrefaction.

Torrefaction, also known as mild pyrolysis, is a thermal process at relatively low temperatures of 200°C to 300°C in the absence of oxygen. Several properties are improved from the point of view of applicability for gasification. For example, the energy density, hydrophobicity and friability are improved. In addition, the grindability is increased as the hemicellulose decomposes, cellulose depolymerises and lignin softens thermally. Furthermore, the cell walls of the biomass are weakened. However, the technology is not yet being used commercially on a large scale. [30]

Hydrothermal carbonisation is a thermochemical process in which raw materials are treated at low temperatures of 180°C to 250°C in an aqueous environment. The products consist of solids, an aqueous solution and small quantities of gases. The main product is hydrochar, which has properties similar to coal and can be easily separated from water due to its hydrophobic properties.

The advantage of the concept lies in particular in the direct usability of feedstocks with a high moisture content. However, this is offset by the high demands placed on the equipment and the need for further research into the optimal process parameters, which depend heavily on the respective feedstocks. [31]

Regardless of the pretreatment selected, the aim for use in entrained-flow gasification is a fine, dry powder ($<200\,\mu$m) that can be conveyed as easily as possible into the reactor. Especially for dry raw materials, torrefaction shows the best compatibility with the process chains under consideration.

Gas Conditioning For downstream processes, the aim is to produce a synthesis gas consisting of CO and H_2. Depending on the intended utilisation, for example as an input for synthesis or as an energy source, the respective ratio between the components differs. In addition to the desired components, the raw gas contains impurities depending on the feedstock used. Thus, gas conditioning is important both for gas purification and for setting the required concentration ratios.

The final downstream application of the synthesis gas influences the required purity of the synthesis gas. In a review, Leuter et al. summarise the required order of magnitude for various components in the synthesis gas depending on the application [32]. Among other things, particulate matter, tars, nitrogen compounds, sulfur compounds, halogens, alkali metals, and heavy metals must be taken into account. In general, lower thresholds must be maintained for energetic utilisation than for biological or catalytic processes.

A brief comparison of gas purification approaches is compiled in [29], from which the following paragraph is taken. Technologically, gas purification is divided into hot (dry) and cold (wet) processes. Although hot gas purification has energetic advantages over cold gas purification, the material requirements and therefore the costs are significantly higher. Cold gas purification processes, which are, for example, marketed under the brand names Selexol® and Rectisol®, are state of the art and are already widely used commercially. Both processes can be used to remove sulphur components and CO_2 from the synthesis gas, whereby additional steps, for example adsorptive beds, may be needed depending on the downstream application.

The H_2/CO ratio can be adjusted using a water-gas shift (WGS) reactor by either increasing the H_2 (forward WGS) or CO (reverse WGS) content of the synthesis gas or by adding hydrogen. Consequently, either the H_2 or the CO yield can be increased by a WGS reactor. Typical ratios range between 2 and 3, which in most cases means a shift towards more H_2 and CO_2. As CO_2 often cannot be used for downstream applications, it is removed in the gas purification step. Consequently, in order to keep carbon utilisation high, current literature often discusses applying the shift towards CO and adding H_2 from water electrolysis, known for example as power- and biomass-to-x. If the shift reaction is applied before gas purification, it is referred to as sour WGS.

2.4.2 Sustainable Feedstock Potentials

The future aim is for biomass, biogenic residues and waste to serve as a more climate-friendly alternative to the use of fossil fuels such as oil, gas and coal. A sustainable system not only optimises the ecological aspect, but also requires economic and social aspects. On the one hand, it is important to consider the quantity and cost of the feedstock that can be provided. Potential studies serve as a data basis here, which differ among other things according to the following characteristics: Spatial extent, spatial resolution, temporal component and potential type (theoretical, technical, economical). On the other hand, the chemical and physical characterisation of the feedstock is important in order to be able to assess whether a feedstock is suitable for a specific application. Typical parameters here are the elemental composition, lower and higher heating value, mechanical processability and the impurities contained, which have an effect on the requirement and expense of gas purification.

Table 2.1 lists characteristic parameters and potentials for a single example from each of the groups biomass, biogenic residues and waste. The values of the elemental analysis and the lower heating value are based on the mean values of analyses from several databases. While biomass and biogenic residues have similar parameters, plastics are characterised by significantly higher hydrogen and carbon contents. The calorific value is also higher. This is particularly due to the significantly less complex structure of the molecules in plastics compared to biogenic cell structures. In Germany, the potential of plastic waste alone is currently in the order of 56 TWh per year, with a strong upward trend. At present, more than half of the waste is utilised exclusively for energy [33]. In contrast, the biogenic potential in Germany is an order of magnitude higher, although a large proportion is already being utilised.

Table 2.1: Characteristic parameters and potentials in germany of different alternative feedstock, each represented by one example.

Parameter	**Unit**	**Biomass**[a]	**Biogenic residues**[b]	**Waste**[c]	**Ref.**
C-content	wt.-% (daf)	50.8	50.7	73.8	[29, 34]
H-content	wt.-% (daf)	6.1	7.1	10.3	[29, 34]
O-content	wt.-% (daf)	42.8	34.5	4.2	[29, 34]
LHV	$MJ\,kg^{-1}$ (daf)	18.9	20.1	35.4	[29, 34]
Potential	$TWh\,a^{-1}$	186.0	280.0	-	[33, 35]
	$Mt\,a^{-1}$	-	-	5.67	

[a] C-/H-/O-content, LHV: untreated wood. Potential: energy crops and wood

[b] C-/H-/O-content, LHV: sludge.

[c] Mixed plastics.

2.5 Power-to-X

As already mentioned in section 2.1, the demand for electricity will rise in the coming years. Thereby, the use of electricity can be categorised into five groups as shown in Figure 2.6, with demand from conventional applications (for example lighting, cooking, IT) and mobility demand alongside heat and gaseous and liquid energy carriers. Conventional electricity demand is assumed to remain constant in the coming years due to a reduction as a result of efficiency-enhancing measures and an increase in digitalisation and IT applications [2]. In addition, demand will increase sharply due to electro mobility [36]. Power-to-x applications can be subdivided into power-to-gas and power-to-liquids, whereas power-to-heat is included in this term not consistently.

Since the synthesis of energy carriers from synthesis gas is equivalent to the biomass-to-x approach, the synthesis processes are described separately in section 2.6. This section briefly summarises the concepts of heat generation from electricity and the production of electricity-based synthesis gas.

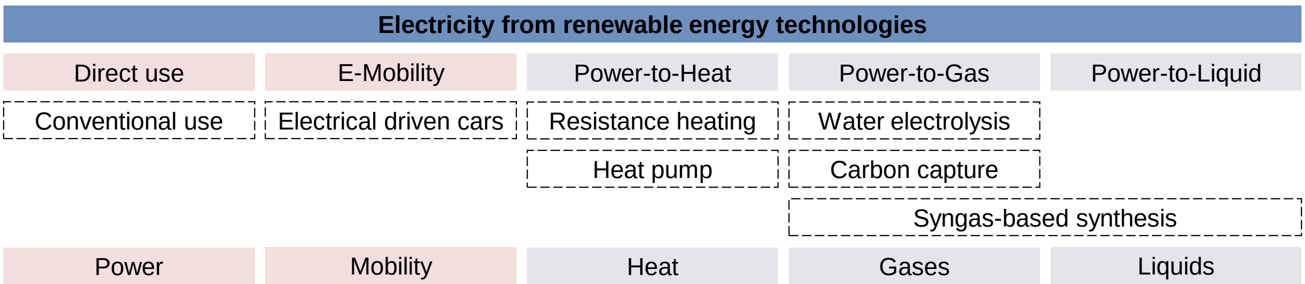

Figure 2.6: Schematic illustration of the potential ways of utilising electrical power for various applications.

2.5.1 Power-to-Heat

Using electricity to provide heat is defined as power-to-heat. Bloess et al. show that, almost regardless of the assumptions in system studies, power-to-heat can be used as a substitute for fossil fuels, supports the integration of renewable energy and, overall, can contribute to decarbonisation [37]. Initially, Bloess et al. distinguish between centralised and decentralised applications, whereby the technologies used in space and hot water heating are primarily heat pumps and resistance heaters. In contrast, from a power-to-heat perspective, high-temperature applications above a certain temperature are limited to resistance heaters or arc discharge, for example. In a system study, Miehling et al. show that in a selected example region, the entire building-specific heat supply and more than 67 % of the high-temperature process heat would be electricity-based [38].

2.5.2 Power-to-Gas

In this case, power-to-gas refers to the supply of gaseous energy carriers before being subjected to further processing or upgrading. While methanisation, which is the synthesis of an energy carrier similar to natural gas, is also categorised under power-to-gas in the literature, only the supply of hydrogen via water electrolysis and CO_2 via carbon capture is discussed here. Further syntheses, which commonly are based on synthesis gas consisting of a H_2/CO mixture, are discussed in section 2.6.

Water Electrolysis The fundamental mechanism of water electrolysis is based on the splitting of water (H_2O) into oxygen (O_2) and H_2. The energy required is generated in the form of electricity and, in some cases, partly as thermal energy. There are three major technological variants of water electrolysis, which are described based on [39], whereas current specific parameters are taken from [40]. The levelised costs of hydrogen in [40] are calculated on the assumption of 7000 full load hours and electricity costs of 100 € MWh^{-1}, with the maximum corresponding to the status quo and the minimum to the 2030 perspective.

- **Alkaline electrolysis:**
  With a TRL of 9, alkaline electrolysis is the most mature technology among the electrolysis variants. Here, the electrodes are immersed in a liquid electrolyte, usually an aqueous KOH solution, and separated by a membrane. Electrons and OH^- ions are used for charge and mass transfer. With an energy demand of 59 kWh kg_{H2}^{-1}, costs of 7.26-6.40 € kg_{H2}^{-1} can be achieved. A purity of 99 % can be achieved for hydrogen and oxygen, whereby the hydrogen purity can be increased to up to 99.999 % by catalytic gas purification. [39, 40].
- **Proton exchange membrane electrolysis:**
  In contrast to alkaline electrolysis, proton exchange membrane electrolysis is based on a solid electrolyte, which allows for a much more compact design. Electrons and H^+ ions are used for charge and mass transfer. Higher hydrogen purities of 99.99 % can be achieved without further purification. At 8, the TRL is currently still slightly below that of alkaline electrolysis. However, from the perspective of the specific energy requirement (52 kWh kg_{H2}^{-1}) and the specific costs (6.66-5.96 € kg_{H2}^{-1}), there are already further advantages of proton exchange membrane electrolysis. [39, 40].
- **Solid oxide electrolysis:**
  Solid oxide cells enable operation at significantly higher temperatures of 700-900°C than in competing technologies. This results in higher efficiencies, although it places particularly high requirements on the materials. While the TRL of 4-7 still reflects a need for development, the technical and economic parameters of 40 kWh kg_{H2}^{-1} and 6.27-5.53 € kg_{H2}^{-1} are promising. Furthermore, the solid oxide cell enables the co-electrolysis of water and CO_2 to H_2 and CO, which can be advantageous, especially regarding further upgrades via syntheses. [39, 40].

Carbon Capture In power-to-x applications, the carbon for further synthesis is provided in form of CO_2 via carbon capture technologies. A distinction is first made between point sources and extraction from ambient air, also known as direct air capture (DAC). Point sources include all process-related emissions, for example from the cement industry, and exhaust gas flows from power plants or waste incineration. Depending on how the CO_2 is used, the entire process is referred to as Carbon Capture and Storage (CCS) or Carbon Capture and Utilisation (CCU). In terms of technology, a distinction is made between absorption- and adsorption-based processes for point sources. In the case of DAC processes, wet and dry processes are used. Table 2.2 briefly summarises current technologies. However, there are already several detailed reviews on carbon capture in the literature, reference is made to these for a detailed description [41, 42].

Table 2.2: Summary of carbon capture technologies, divided into point sources and direct air capture. Directly taken from [43].

Method	**Description**
Capture from point sources	
Absorption technologies	CO_2 is removed from flue gases by absorption in liquid solvents. Typically aqueous amine solutions are used and water-soluble salts are formed in the process. Afterwards CO_2 can be recovered in a desorption column.
Adsorption technologies	Solid adsorbents are used for the CO_2 capture. Typical adsorbents are carbons, alumina, silica and zeolites but also new adsorbents are investigated e.g. polymers. Cyclic processes are implemented for the loading and regeneration of the adsorbents in particular pressure vacuum swing adsorption and temperature swing adsorption. Furthermore, so-called carbonate looping processes, which are based on chemisorption can be used. The most prominent process is calcium looping (using CaO as sorbent). CO_2 is captured forming calcium carbonate. The sorbent is afterwards regenerated via calcination releasing the CO_2.
Direct air capture	
Wet air capture	CO_2 from ambient air is absorbed in a liquid solution within packed-columns, convection towers or spray-tower contractor systems. An example is the soda/lime process based on a sodium hydroxide solution.
Dry air capture	Typically solid organoamine based adsorbents are used for the CO_2 capture. Desorption occurs at elevated temperatures in an inert gas stream, however only a diluted CO_2 stream is generated. Newer developments focus on improving regeneration conditions.

However, several aspects have to be addressed to fully define the optimal utilization of power-to-gas processes in future energy systems. These include, for example, the choice of water electrolysis technology or the costs of hydrogen supply and the carbon source. To the same extent, flexibility or a dynamic operation as well as the respective downstream process design is still ongoing research.

2.6 Synthetic Energy Carriers

Besides H_2, the most frequently discussed synthetic energy carriers in the literature are: methanol (MeOH), dimethyl ether (DME), Fischer-Tropsch (FT) syncrude, synthetic natural gas (SNG) and ammonia (NH_3). What they have in common is that they are already produced from fossil-based synthesis gas and can therefore be easily adapted to sustainably supplied synthesis gas. These can be either electricity-based (power-to-x) or solid feedstock-based (biomass- or waste-to-x). However, a distinction must be made as to whether carbon is provided in the form of CO or CO_2. Since only catalytic processes are considered in the content of this dissertation, the reader is invited to refer to the relevant literature on, for example, biological routes [44].

The graphical comparison of synthetic energy carriers in Figure 2.7 a) demonstrates the storage and transport problems associated with gaseous energy carriers such as synthetic natural gas (SNG) and hydrogen (H_2). However, these can also be liquefied at the cost of energy consumption. With the exception of NH_3 from electrolysis hydrogen, a comparison of the elementary composition in Figure 2.7 b) shows that none of the products directly resembles the composition of the starting products such as biomass. This inevitably leads to losses or the need to add H_2 from an additional source.

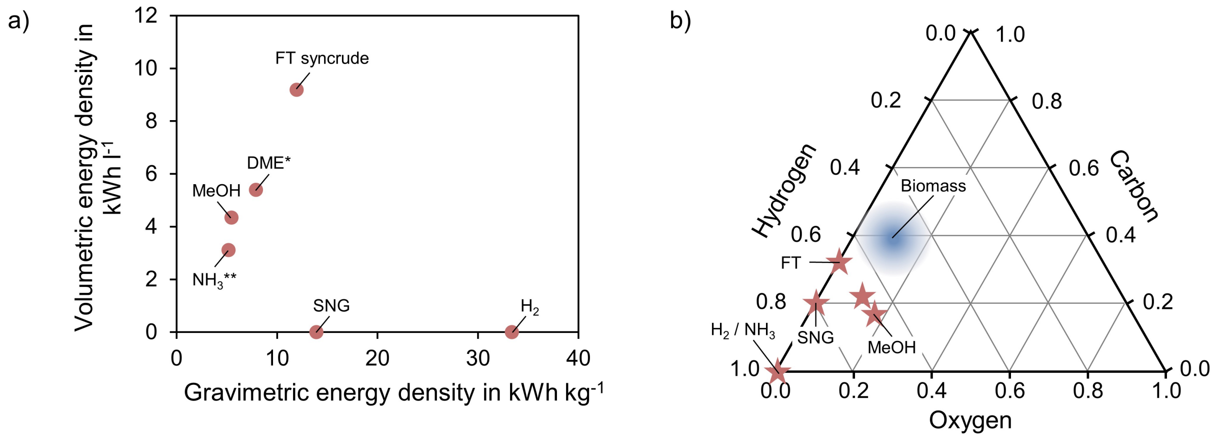

Figure 2.7: Comparison of the synthetic energy carriers H_2, MeOH, DME, FT syncrude, SNG and NH_3 regarding the volumetric and gravimetric energy density (a) and the molar content of H, C and O. Own illustration of data taken from [29, 43]
*DME at 10 bar, **NH3 at 8 bar

2.6.1 Methanol (MeOH)

Based on a high-pressure and high-temperature process, MeOH is produced on an industrial scale since the early 1920s. Nowadays a low temperature (200 °C-300 °C) and low-pressure (50 bar-100 bar) process is used exclusively. Typically, commercial catalysts based on CuO and ZnO, with additional stabilizing additives, are used achieving over 99 % selectivity. The H_2/CO and H_2/CO_2 ratios are 2 and 3, respectively, with slightly higher ratios tending to improve the process. The variety of existing large-scale converter designs extends up to scales of several kilo tons per day. The converter designs mainly are dominated by fixed catalyst beds, which are cooled to achieve an isothermal temperature profile. To meet desired purity levels, product upgrade steps are needed, mostly consisting of distillation processes. Current research on methanol synthesis aims at advanced catalyst and reactor designs, flexible and dynamic operation as well as economic analysis. To reduce the demand for hydrogen storages without losing flexibility options, converters have to be able to be operated in part-load without harming, for example, the catalyst. This is claimed by various producers to be possible, at least in a defined range of operation. Overall, the integration in the overarching energy system is the key to an economic and ecological utilization in future energy systems. [43]

2.6.2 Dimethyl Ether (DME)

Industrial DME synthesis currently relies on a two-step process with methanol as intermediate product. There is, however, the possibility of a one-step DME production, in which the combined appearance of MeOH formation, WGS reaction and MeOH dehydration lead to a higher syngas utilization compared to the MeOH synthesis. The operation conditions of direct DME syntheses are comparable to those of MeOH with temperature ranges between 200 °C-300 °C and pressure between 30 bar-70 bar, while the two-step process is operated between 220 °C-400 °C and 1 bar-30 bar. The stochiometric syngas ratio of H_2/CO_2 is 3. For a direct production of DME, hybrid catalysts are used combining methanol formation and dehydration reactions. However, most of the current large scale DME plants are using the two-step process due to economic reasons. The product upgrade in the two-step process typically consists of a two-column distillation, separating DME from light ends (which can be used as fuel gas) and unconverted MeOH and water. The one-step upgrade process however is more complex, as the product stream contains a broader spectrum of components, for example CO_2. Studies on the flexibility or dynamic operation are still missing, as well as extensive techno-economic evaluations. However, existing publications agree on much higher costs per ton DME via power-to-DME than based on biomass or coal gasification. [43]

2.6.3 Methane or Synthetic Natural Gas (SNG)

Compared to other fossil fuels, natural gas has the lowest specific greenhouse gas emissions, which is why it is currently seen as the last fossil fuel during the energy transition. The use of natural gas extends to the production of electricity and heat as well as a feedstock for the (chemical) industry. Natural gas consists largely of methane, which can be produced synthetically using several processes and is known as SNG. In the future, SNG will primarily be seen as a possible storage medium in long-term storage facilities and as a feedstock for individual industrial processes. The process pathways, most of which are already mature, utilise both fossil and sustainable feedstocks (biomass, waste, CO_2, H_2) and are established as both thermochemical and biochemical pathways. With a high technology readiness level and already applied on a large scale, Haldor Topsoe's TREMP process is one of the standard processes for the thermochemical synthesis of methane. The methanation process is divided into three reactors, which are operated adiabatically between 250 °C and 600 °C. Nickel-based catalysts are used to facilitate the exothermic reactions. After the third stage, sufficient quality SNG is available for feeding into today's natural gas networks. [29, 45]

2.6.4 Fischer-Tropsch (FT) syncrude

In contrast to the previous listed synthesis, FT synthesis has a broad variety of hydro-carbons of different chain-length as products. FT synthesis can be used both for fuel and wax production, where the fuel fraction, for example, can be used as direct diesel or gasoline substitute. The desired reactions are limited in temperature and pressure by coke formation and short chain-length formation as upper bound and reaction velocity and conversion rate as lower bound. Typically, a H_2/CO ratio of 2-2.2 is used in combination with Fe or Co catalysts. The temperatures range between 300 °C-350 °C for high temperature FT synthesis and between 200 °C-250 °C for low temperature FT synthesis. The products chain-length can be described by the Anderson-Schulz-Flory distribution, which is a function of temperature, pressure and syngas composition, as well as the used catalyst. Low-temperature reactors favor liquid hydro-carbons and waxes, whereas high-temperature reactors mainly produce alkenes and gasoline. Based on the desired market, the product mixtures can further be upgraded. They can either be used to produce waxes (for example by hydrogenation or hydro-isomerization), or converted to short chain length via hydrocracking. All of those processes are well known from the petrochemical industry. As current studies state, biomass or other solid feedstock based liquification processes tend to have lower specific productions costs compared to power-to-liquid processes. However, they do not consider the limited potential of the respective feedstock or other limiting indicators. This complex coupling effect still has to be evaluated, to identify the market opportunities of FT products in future energy systems. [43, 46]

2.6.5 Ammonia (NH_3)

Accounting for 1-2 % of global energy demand and around 1.6 % of global CO_2 emissions, NH_3 production has a significant presence in the global balance. The main application of NH_3 is fertiliser production. With over 90 %, the largest share of the world's NH_3 demand is produced using the Haber-Bosch process. Herein, H_2 and N_2 are reacted to form NH_3. The synthesis takes place at temperatures between 400 °C and 500 °C and at pressures above 100 bar. Iron-based catalysts are used. The product is finally separated as a liquid phase by cooling the product gas to cryogenic conditions (-20 °C). Compared to other fossil feedstock, natural gas is both technically and economically the most favourable to produce the synthesis gas. In addition to H_2, which can be provided in future energy systems via sustainable paths such as water electrolysis or from biomass, N_2 is the second component, which is provided from air separation plants. [29, 47]

3 Research Demand, Objectives and Methods

The objective of climate protection through the transformation of energy systems into fully sustainable circular economies is no longer merely a topic of scientific debate; it is increasingly being embedded in law as a binding goal of our society. Many questions that still need to be answered in order to make the investments required for a successful transformation are being discussed from different perspectives. The difficulties arise in the diversity of stakeholders, the uncertainties in developing individual technologies and the uncertainty of future, non-technical boundary conditions.

The partially criticised choice of hydrogen as the energy carrier of the future in the early 2020s has defined the first boundary conditions but has also opened up new questions. One of these questions relates to future carbon sources. If sectors with demand beyond purely energetic utilisation are considered (for example the chemical industry), the demand is expanded by the factor of material supply (for example basic chemicals).

One area that deals with the sustainable supply of energy systems is utilising (biogenic) residues in so-called biomass-to-x processes. The aim is to produce a synthesis gas from sustainable feedstock that can be used in conventional applications such as the synthesis of chemicals and fuels. Biomass-to-x is researched and further developed by a large community of scientific institutes and by the industry. Accordingly, there are a large number of potential process routes. However, there is no clear choice of one optimal process. Rather, changing boundary conditions lead to the selection of different processes.

The aim of this dissertation is to analyse the factors influencing the technology benchmarking process at both the process and system level, with an explicit focus on the discussion of the method. For this purpose, the entire process of plant modelling up to system integration is elaborated using the example of an entrained flow-based biomass-to-x plant. The example is chosen to discuss the method, without explicitly focussing on the presentation of the plant. This ultimately makes it possible to set up an exemplary energy system model in which the chosen biomass-to-x plant is implemented according to the techno-economic analysis and enables an evaluation of the major influencing factors on the technology benchmark from both a system and a process perspective. This will allow recommendations to be made on how energy system models should be designed and applied when used for the evaluation of novel technologies.

A detailed technology benchmarking can be subdivided into the following research questions and the associated scientific methods. This also corresponds to the structure of this dissertation:

1. **What are the current and expected boundary conditions of energy systems?**
   As shown in section 2.1, a lot of energy system studies are published on a variety of topics, but an analysis of the similarities and differences is still missing. To determine the current status and currently expected developments a meta-analysis of existing system studies is carried out. By focusing on the energy transition in Germany, the question whether decentralised or large-scale process or power plants are needed is answered.
   → Meta-analysis in **Article I**
2. **What affects the selection of the biomass-to-x product on a technical level?**
   The aim here is a direct comparison on the energetic/technical level. As can be seen from the literature research, so far only single process variants or individual products have been investigated. By modelling six different synthesis variants at an identical level of detail, a direct comparison of the products is possible, which until now is missing in literature.
   → Process simulation in **Article III**.
3. **How does the chosen biomass-to-x product influence the plant costs?**
   Additional to the solely technical analysis, a comparison of different biomass-to-x products on an economic level is lacking in literature as well. Building on the modelling, it is thus possible to assess at a market level which products already can be produced competitively today. Furthermore, the combination of technical and economic parameters can be used as an input for an analysis from a system perspective.
   → Techno-economic assessment in **Article IV**
4. **What are the system variables that influence technology utilisation the most?**
   Based on the literature analysis, it can be seen that the discussion of uncertainties in energy system analyses is becoming increasingly important. While more and more work is being published on the explicit calculation of uncertainties, there is still no analysis of the most influential factors. On the one hand, these factors are generally important for the development of energy system models; on the other hand, they can be used to identify the parameters that are most important for the design of new types of plants (for example biomass-to-x) from a system perspective.
   → Energy system optimisation in **Article V** and **Article VI**

Finally, the combination of the aforementioned individual analyses enables a holistic discussion. The aim here is, among other things, to compare the identified influencing factors from the different perspectives. The findings of the meta-study and the technical and economic analyses at the process level are integrated into the evaluation at the system level. Furthermore, the method as a whole will be discussed in **Chapter 7**.

The aim of this dissertation is therefore initially to **analyse a biomass-to-x concept at process level**. Subsequently, the utilisation of the example process will be **evaluated from a system perspective** and the main **factors influencing its utilisation will be identified**. Finally, the approach of benchmarking new technologies from a process and system perspective will be **summarised in a consolidated discussion, focused on the method**.

4 Methods

Six articles have been written to discuss the research question formulated in chapter 3. Methodically, **Article I** is a meta-analysis and thus a solely literature-based study placed in chapter 2. The general term of energy systems can be used for systems on a process level, for example biomass-to-x processes, and for systems on a macro-economic perspective, for example the German energy system. To clearly distinguish between the two perspectives and, thus, between the two fundamentally different modelling approaches, their differences are discussed in section 4.1, and the nomenclature used in this study is defined. In section 4.2 the method of process modelling is described as used in **Article III** and in section 4.3 the assessment of economic process evaluation is summarised as used in **Article IV**. The method of modelling overarching energy systems used in **Article V** and **Article VI** is presented in section 4.4. Finally, in section 4.5, a summary of the energy system model framework *OpTUMus*, which has been published in **Article II**, is presented.

4.1 Differentiation between Energy System and Process Modelling

The term energy system describes all levels of systems used to generate, supply, transport or store energy, or the combination of such systems. Since such systems are becoming increasingly complex and innovative concepts are often too expensive to test in demonstration plant sizes, using energy system models or digital twins is becoming increasingly common. Additionally, not only power and heat are considered within energy systems, but all kinds of energy carriers are summarised under energy systems. Subramanian et al. suggest that such models can be classified either by their basic type of modelling (physical, mathematical or computational) or by the level of aggregation, which is linked to more characteristic parameters [48]. The latter recommendation is chosen to distinguish between process and macroeconomic levels in this study. Thus, the evaluation of all parameters directly connected to the assessed process is referred to as process modelling and the techno-economic assessment. On the other hand, all factors influencing the overarching system are allocated to energy system modelling.

4.2 Process Modelling

Computer models are used to analyse, compare and optimise processes without an actual experiment or demonstration plant. These models can simulate the physical and chemical behaviour of process plants on a utility level, which is often enough to compare new process concepts to existing ones or to optimise them on an energetic and technical level. According to [49], those models mainly consist of:

- A process flow diagram including all utilities, components and streams
- An energy and mass balance

Depending on the current development status, the aimed level of detail can vary from simple block diagrams to detailed process flowsheet diagrams, including piping and instrumentation (also referred to as P&ID) [50]. While block diagrams, for example by combining utilities into overarching groups, are satisfactory enough to discuss the overall concept of a process, an actual energy and mass balance for each subsystem needs at least a process flow sheet diagram including all main components and streams. Standardised pictograms are used for common components in process flow diagrams to simplify readability. However, company-specific variants are sometimes also used. As stated in [50], the essential information to be listed in a process flow diagram includes all process equipment and all stream information (composition, temperature, pressure, enthalpy and flow rate). An exemplary block diagram is shown in Figure 4.1, representing a biomass-to-x plant as evaluated in chapter 5.

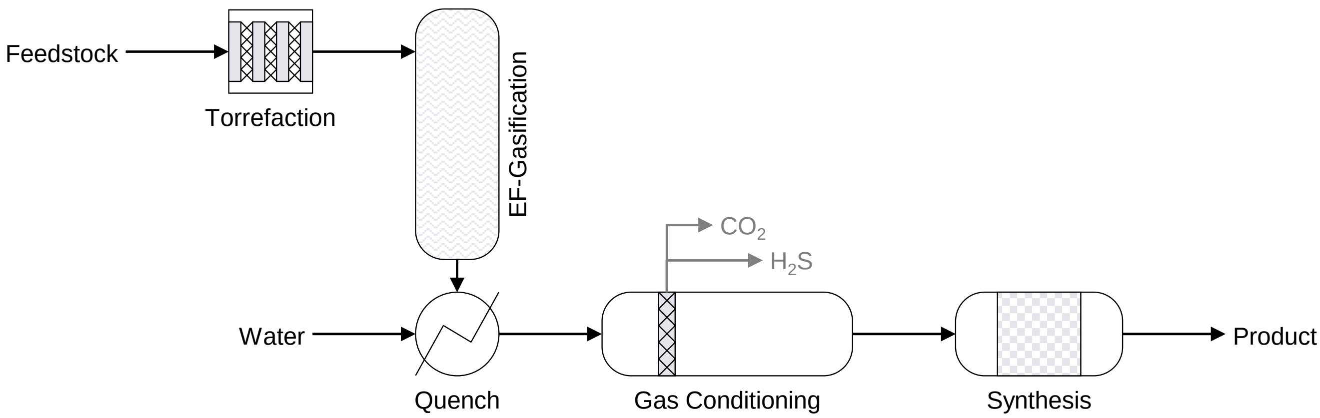

Figure 4.1: Exemplary block flow diagram of a biomass-to-x process, based on entrained flow gasification.

The required level of detail of the results from the process simulation is always determined by the following application of the data. In the present work, the data is required to enable a cost estimate of the plant (more on this in section 4.3). Then, the technical and economic parameters are used to integrate the system into an energy system model. Both applications require at least sizing of the main components, whereby, for example, the piping and all equipment for control systems do not have to be configured. Additionally, the energy system model needs balances for all in- and outgoing streams.

Each process component has specific properties related to the incoming and outgoing streams. This includes both thermodynamic/physical state changes and chemical reactions. The energy and mass balances of the entire process are calculated by solving all equation systems under given boundary conditions, for example at standard conditions. Nowadays, proprietary software is used for both the flowsheet design and the calculation of the equation systems [49]. On the one hand, these software packages offer a graphical user interface to make it easier to create flowsheets based on standardised pictograms. Furthermore, they contain all common process components, including their equation systems. Additionally, various property methods that can describe the thermodynamic and physical behaviour of the evaluated gases and liquids are also included. It is further differentiated between steady-state and dynamic simulations. In the present work, the analysis of transient states is not included, which is why steady-state models are sufficient.

In this study, Aspen Plus®[1] is used for all process models (process flow diagrams and calculations). Process modelling is used for the evaluations in chapter 5, to model different variants of a biomass-to-x process plant containing:

- Pretreatment (torrefaction)
- Gasification (entrained flow gasification incl. full water quench)
- Gas conditioning (sour water gas shift and acid gas removal)
- Synthesis (synthesis of different products including MeOH, DME, FT syncrude, NH_3, SNG and H_2)

Detailed descriptions of the processes as well as the state of the art and the used process variants can be found in in the respective publications **Article III** (section 5.1) and **Article IV** (section 5.2). In addition to the technological components, the choice of feedstock also has a major influence on biomass-to-x plants. The input data required here are:

- Proximate analysis (moisture, fixed carbon and volatile matter)
- Ultimate analysis (elemental analysis)
- Lower/higher heating value

These data are not generated in the present work itself but are taken from existing fuel databases and previous publications by other authors. **Article III** (section 5.1) describes the selection of the generic feedstock used in more detail.

In summary, the result of the process modelling is a process flow diagram of the plant with all required main components. The respective description and scaling of the main components are also included. The balancing of the mass and energy flows includes performance indicators such as the energetic efficiency, carbon and hydrogen conversion rate as well as the temperature levels of the supplied and discharged heat, and the demand for auxiliary energy (for example electricity).

[1] Aspen Plus® V12 by Aspen Technology, Inc. (Aspen Tech Website).

4.3 Economic Assessment

Various approaches can be found in the literature for estimating the costs of process plants. The names and definitions of the individual approaches differ depending on the institute or company and individual applications. However, according to Peters et al., these can be categorised into five groups [51]:

1. **Ratio estimate:** Accuracy of ±30 % by scaling the costs of existing, similar projects to the aimed process scale
2. **Factored estimate:** Cost estimation based on the major process items by using multiplication factors to take all additional equipment into account (accuracy of ±30 %)
3. **Preliminary estimate:** Based on preliminary and limited data, but without final engineering (accuracy of ±20 %)
4. **Definitive estimate:** Detailed flow diagrams but no final drawings and specifications (accuracy of ±10 %)
5. **Detailed estimate:** Based on final engineering including site surveys and final specifications (accuracy of ±5 %)

Next to Peters et al., the work of Towler and Sinnott summarises the commonly used methodology in a comparable extensive way [51, 52]. However, in this work the approach described by Peters et al. is used.

The different levels of cost estimation approaches 1 to 3 can be summarised as predesign cost estimates, which are especially important as they are used to decide whether a new concept is further developed or not, based on rough preliminary data [51]. In this study the factored estimate approach is used, as the information available from the process simulation (see section 4.2) lays between the requirements of approach 2 and 3. Thus, the results in section 5.2 have to be interpreted with an accuracy of around ±30 %.

For estimating the capital investment different methods with varying levels of detail can be used. The chosen approach uses the cost of all main components (for example reactors, pumps, compressors) as a basis for estimating further direct and indirect costs. Figure 4.2 shows an overview of the cost structure.

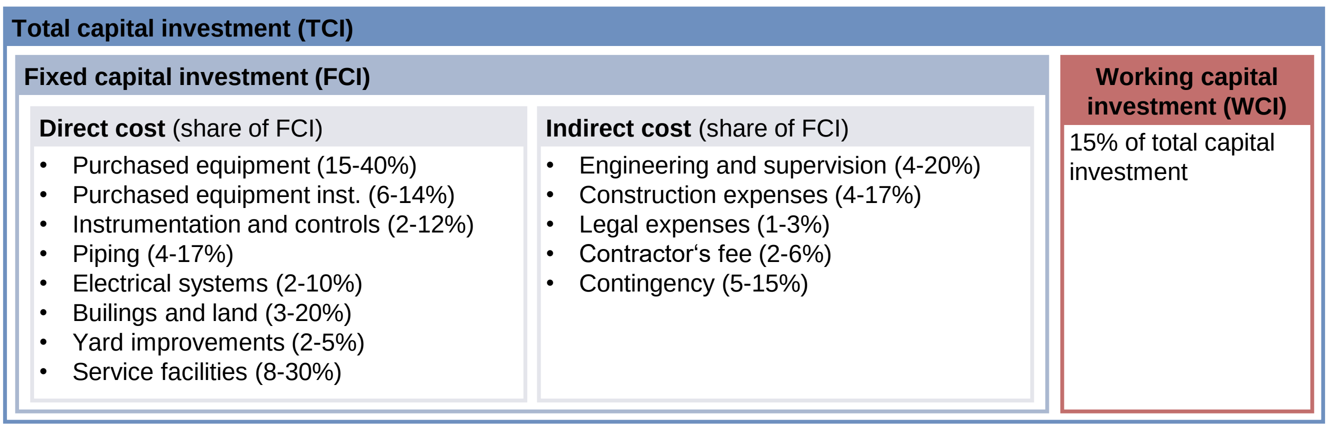

Figure 4.2: Overview of the factor based estimation of the total capital investment, based on [51].

The shown range for the share of each cost component for calculating direct costs (for example piping, buildings) and indirect costs (for example engineering, legal expanses) are collected based on an extensive literature and industry review for various types of process plants in [51]. For each sub system the actual chosen value within the given range depends on the process complexity and the handled materials (for example solid vs. fluid).

Most of the factors used for estimation relate to the cost of purchased equipment. Two approaches can be used here: Scaling of existing component prices or cost functions (fitted cost curves to actual cost data). Both approaches are used in this paper. The reason for this is that good cost correlations only exist for standard components such as heat exchangers, compressors and pumps. Both the correlations implemented in the process simulation software used (for example APEA[2]) and literature-based correlations (for example [51, 52]) can be used here. In contrast, such correlations are lacking for specific subsystems such as the reactor for entrained-flow gasification or pretreatment via a torrefaction. For this reason, cost correlations are used in this work for standard components and literature values for all other main components. In order to ensure that the literature values provide a significant database, several sources are used and the mean value is calculated, disregarding outliers.

Finally, the specific product costs can be calculated in order to compare the new process with the given market conditions. An overview of the components of the total product costs can be seen in Figure 4.3. The calculation using a factor-based approach can only be used in part here. A distinction must be made between costs that are incurred independently of any production (rent, salaries, financing of capital) and costs that are required per unit of the product (feedstock, energy). The respective shares can be determined in part via factors (for example insurance, taxes, depreciation). Costs for feedstock, salaries and energy must be based on the local boundary conditions. On the basis of a large collection of data, Peters et al. have developed an estimate for individual factors as well as for the overarching shares (shown in Figure 4.3) [51].

A more detailed summary of the methodology of a cost estimate using the example of a biomass-to-x plant is summarised in [53]. Whereas the specific factors used in this work can be found in **Article IV**.

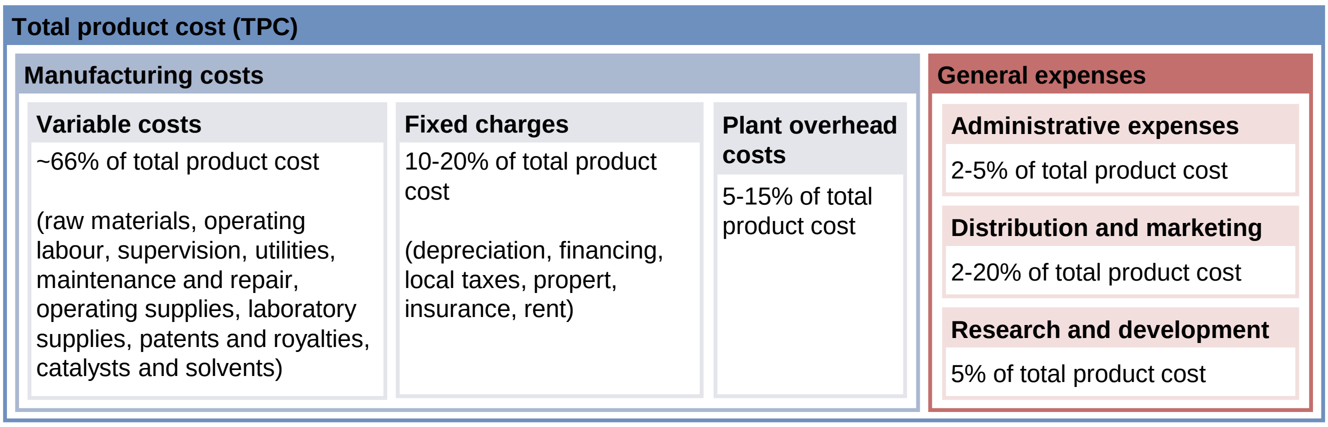

Figure 4.3: Overview of the factor based estimation of the total product cost, based on [51].

[2] APEA: Aspen Process Economic Analyzer; part of the used process simulation software Aspen Plus®

4.4 Energy System Modelling

In addition to the distinction between process and energy system level (see section 4.1), the terminology within energy system modelling is also not uniformly defined in some cases. The computer-aided modelling of energy systems can be divided into three steps: the modelling framework, the energy system model and the solving of the modelling problem (see Figure 4.4). As Suganthi et al. [54] summarise in their review, a large number of modelling approaches are currently known and used. However, the choice of framework already has an influence on the type of model used and the solution approach. As the approach in this thesis primarily can be referred to as an optimisation problem, the reader is referred to the respective literature for further model and solution approaches.

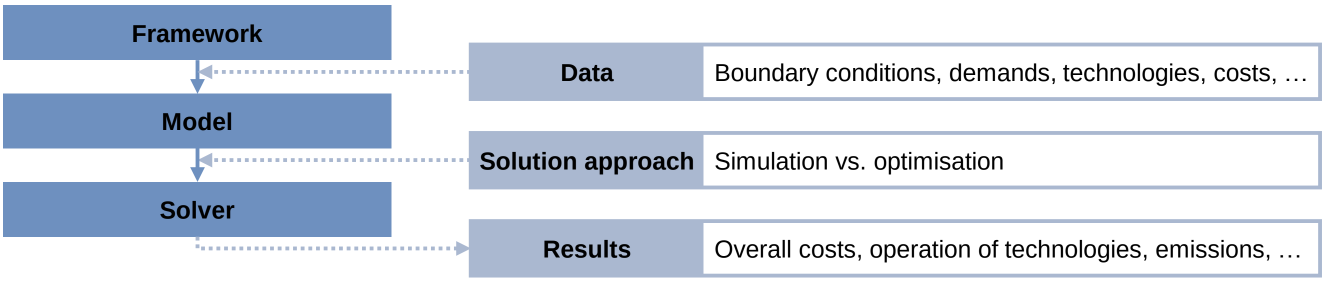

Figure 4.4: Simplified scheme of the approach used for modelling energy systems.

4.4.1 Framework

In purely formal terms, a modelling framework is the mathematical description of all system components of a system and their ability to interact with each other. In the case of energy system analysis, this refers to the implementation of physical and thermodynamic boundary conditions in a software environment and the capability to describe technologies and energy flows within it. This also includes the possibility to solve an optimisation problem or simulate a scenario. According to a survey conducted within the German energy system analysis research network [55], PyPSA [56] and oemof [57] are among the most widely used frameworks, closely followed by in-house modelling frameworks from individual institutes. A description of the framework used in this study can be found in **Article 2** (section 4.5).

4.4.2 Energy System Model

An energy system model is the application of a framework to a specific system, for example the German energy system, and, therefore, describes all included technologies for energy supply, transport, conversion and utilisation. All boundary conditions, for example the weather, and the demand side, for example electricity and heat, are also part of an energy system model. Subramanian et al. differentiate energy system models into *Bottom-Up*, *Top-Down* and *(Demand and Supply) Forecasting* models [48]. While the last one mainly is used to describe the development of potentials based on historic data, Bottom-Up and Top-Down models are more focused on the actual interaction between different primary energy sources, various demands and the respective utilization of technologies. The model used in this work contains both, properties from Bottom-Up and Top-Down approaches. First, from a Bottom-Up perspective, detailed descriptions of technologies are used to describe their optimal operation in future energy systems. On the other hand, as common in Top-Down approaches, the inter-sectoral dependencies of various demands and supplies are modelled.

The range of the required data extends from technological parameters such as conversion efficiencies, degradation and load change behaviour to variable and fixed costs. Furthermore, weather data and projections of energy demand are required. In general, not all parameters are available in the same quality. In this context, among other things, data quality is understood to mean the level of detail of the cost estimate, the origin of the technical parameters (modelling or measurement on demonstration plants) and the year or time of publication. For instance, there are databases in which freely accessible technology data is compiled (for example by the Danish Energy Agency [58] or the U.S. Department of Energy [59]). However, these databases are often insufficient, especially for innovative processes, and individual cost estimates must be used. The data basis of the models used in this study can be found in the respective publications (**Article V** and **VI**).

For the specific case of biomass-to-x plants, which are analysed in the first part of this dissertation, the data is taken from the techno-economic evaluation. The plants themselves are reduced to black boxes for the energy system model. For this purpose, the following data is extracted from the process models and cost estimates for each subsystem (see Figure 4.1):

- Balance of all incoming and outgoing flows (incl. feedstock, products, emissions)
- Energy balance
- Costs (investment costs and variable costs)

According to Lund et al., the actual use of an energy system model can be divided into simulation and optimisation approaches [14]. However, since the literature often refers to model results, the differentiation from model to optimisation/simulation is often smooth.

4.4.3 Optimisation vs. Simulation

The fundamental difference between simulation and optimisation lies in the intended research question. According to Lund et al. [14], simulation is used to analyse a given system. The composition of the technology park is specified accordingly. In contrast, optimisation is used to determine the optimal configuration of a system under given boundary conditions. Although both approaches, as well as combined approaches, can be found in the literature, a meta-study shows that optimisation of energy systems is the most commonly used approach [2]. In this work, the optimisation approach is chosen, whereby aspects of simulation are used in part when it comes to evaluating the operation of new plant technologies.

Problem formulation According to Steck [60] and Martins [61], the optimisation approaches can mainly be categorised into three types: discrete and continuous, linear and non-linear and convex, and non-convex problem formulations. The choice between those formulations is based on the requirements of the model. For example, fixed pipe diameters in district heating systems or start-up/shut-down of individual power plants are modeled as integer or binary variables. However, the computational effort for integer problems is significantly higher. In continuous models such variables can only be approximated. In this work, a linear continuous convex formulation is used in order to reduce the computing time. The choice of a non-discrete formulation is a valid, as the aggregation level is large enough to be be not dependent on discrete effects.

Objective function If the solution approach is optimisation, an objective function is specified, which is minimised using a solver. A common approach in energy system modelling is to minimise the total costs, as this can be interpreted as the macroeconomic optimum. Multi-objective functions can also be used, for example to define the total costs and emissions of the system together as the objective of the analysis.

Solver Solvers are optimisation algorithms and/or heuristics that can be used to solve the formulated problem. Here, commercial solvers such as Gurobi [62] and CPLEX [63] are particularly well known. By continuously developing the algorithms and applying heuristics, these offer performance advantages over other solvers [62, 63]. Due to the user environment of IBM for the application of the CPLEX algorithm, which was available free of charge for scientific purposes at the time of writing, the optimisation problems used in this thesis were solved completely with CPLEX.

4.4.4 Interpretation of Energy System Optimisation Results

Optimisation results must always be interpreted in the context of the used methodology and the respective boundary conditions and assumptions. The single-objective optimisation approach used in this work to minimise the total system costs corresponds to the most widely used approach [64]. Therefore, the result of the optimisation corresponds to an energy system that is the most cost-effective from a macroeconomic perspective. The actions of individual stakeholders within the system, for example to maximise their own profits, cannot be represented in this way. Another point of criticism is that even near-optimal results can lead to strongly divergent results [65]. This is why, for example, Trutnevyte recommends using several near-optimal results to increase the significance of the result [65]. The results of the optimisation essentially consist of the compilation of all technologies and the respective scaling required for energy supply, storage, transport and conversion. In addition, there is a temporally and spatially resolved energy and mass balance that reflects, among other things, the operating behaviour of the technologies. Besides the evident data, other system parameters can also be read from the optimisation results, which can be used for interpretation. In this work dual values and reduced costs are used.

Shadow prices The cost of electricity in the current EU electricity spot market is determined by marginal costs. These are defined as the costs required for the last unit needed to cover the demand. The entire market therefore follows the costs of the most expensive unit sold. These marginal costs can be determined using linear programming via so-called dual values [66]. The dual variables (also known as shadow prices) correspond to the increase in the target function (in this case total costs) when demand is increased by one infinitesimal unit, thus the shadow price is related to a constraint [67], for example energy demand must be the same as the energy supply. In this way, both the electricity production costs and the costs for the supply of energy carriers, for example methanol, can be estimated.

Reduced costs In contrast to shadow prices, reduced costs refer to a decision variable [67]. In this case, the value can be described as the difference between the specific costs of the optimal (chosen) technology to be used to cover the demand and the examined technology that is currently not being used. The value can therefore be interpreted as the amount by which the unused technology would have to be cheaper in order to be utilised.

4.5 Energy System Optimization using (Mixed Integer) Linear Programming (Article II)

The following section serves as a summary of the results of the in section A.2 attached article. The contents of this section were published in:

Sebastian Miehling*, Andreas Hanel*, Jerry Lambert, Sebastian Fendt, Hartmut Spliethoff (2023): Energy System Optimization using (Mixed Integer) Linear Programming. In: arXiv. doi:10.48550/arXiv.2308.01882

*Dual-first authorship, both authors contributed equally to this work.

Summary This article presents a set of equations to build an energy system model. The term energy system is used to describe the combination of all energy supply systems (for example electricity and material energy carriers), transport, and all energy sinks (demand such as electricity, heat and mobility). The scale considered here generally covers large areas of one or more countries. Typically, the modelling of energy systems aims to compare different scenarios characterised by changing boundary conditions and assumptions. Linear programming is commonly used in the literature, with or without the possibility of mixed-integer expansion. The same mathematical formulation is used in this work. However, the framework also aims to describe the operation of individual components of the energy system, such as power plant units, in detail.

Nodes and edges are introduced to describe the supply, transport and demand structures. All energy sources are referred to as nodes. In contrast, all technologies for converting energy into other types of energy (for example electricity into heat) and transporting energy are defined as edges. The fundamental physical laws of energy and mass conservation apply to all nodes and edges. If these basic equations are extended, technological properties such as start-up processes, storage systems or dependencies between several edges can be added. Introducing mixed-integer formulations allows the model to consider block-sharp start-up and shut-down processes of systems and other integer variables, such as the number of pipelines required. In the next step, the combination of the physical model with economic cost functions is extended. This allows to minimise the energy system according to the overall economic costs. This is considered a standard objective function in the optimisation of energy systems. The decision variables, i.e. the variables that can be varied to find a solution, usually include parameters such as the composition of the technology portfolio, the respective plant size and the utilisation planning of the plants themselves. For the planning of operations, it is therefore possible to define time-dependent variables and thus consider seasonal changes in conditions, for example, weather phenomena or demand time series.

Finally, a simple example of an energy system model is presented, representing the concept of the models used in chapter 6 in a highly simplified version.

Contributions This paper is the result of the common effort of more authors. **Sebastian Miehling:** Conceptualisation, Methodology, Software, Validation, Visualisation, Writing - original draft. **Andreas Hanel:** Methodology, Software, Validation, Visualisation, Writing - original draft. **Jerry Lambert:** Software, Validation, Writing - original draft. **Sebastian Fendt:** Project administration, Writing - review. **Hartmut Spliethoff:** Supervision, Writing - review.

5 Process Evaluation using Process Modelling

The analysis of new processes usually involves two steps. First, a technical and energetic evaluation of the process is conducted. Then the process is evaluated in terms of economic indicators. This method is shown in this chapter on the example of entrained-flow gasification based biomass-to-x processes. The method is divided into section 5.1, presenting the technical and energetic part, and section 5.2, the economic evaluation. Those two articles have been planed as a two-part publication and thus consider the same process concepts.

5.1 Entrained Flow Gasification-based Biomass-to-X Processes: An Energetic and Technical Evaluation (Article III)

The following section serves as a summary of the results of the in section A.3 attached article. The contents of this section were published in:

Andreas Hanel, Vincent Dieterich, Sebastian Bastek, Hartmut Spliethoff, Sebastian Fendt (2022): Entrained flow gasification-based biomass-to-X processes: An energetic and technical evaluation. In: Energy Convers. Manag. doi:10.1016/j.enconman.2022.116424

Summary This article contains an extensive comparison of biomass-to-x processes. By using steady-state process models built in Aspen Plus®, various product routes based on entrained flow gasification of an exemplary feedstock are compared. Both energetic and technical, as well as material-based key performance indicators, are used. The considered products are ammonia (NH_3), methanol (MeOH), dimethyl ether (DME), Fischer-Tropsch (FT) syncrude, synthetic natural gas (SNG) and hydrogen (H_2) (with and without carbon capture).

All processes are subject to the same boundary conditions and basic configuration of the biomass-to-x plant to guarantee comparability. The reference feedstock (beech wood chips) is prepared as a powdered feedstock for the entrained flow gasification via torrefaction and grinding. The gasification itself takes place under an oxygen atmosphere, followed by a full water quench, as well as a multi-stage synthesis gas conditioning via Selexol scrubbing and a water gas shift reactor.

Finally, the respective product synthesis follows. All steps are included in the process model, although the individual models differ in heat integration and the synthesis gas composition required in each case. The process scale is defined by a $100\,MW_{th}$ feedstock input to the gasifier.

The energetic evaluation shows that the selective processes have comparable fuel utilization efficiencies of around 60 %, whereas those of the non-selective processes, for example 40 % for FT, are significantly worse. NH_3 also shows a worse energy yield of 42 % due to the additional nitrogen requirement and the exclusive use of hydrogen. In total, all processes are exothermic, whereby a consideration of the temperature levels at which the waste heat occurs is distinctly different. For example, FT could be the most promising process, for example in an industrial area, if both light-ends and waste heat are integrated.

Carbon and hydrogen conversion are of particular interest in terms of material balances. Since all considered synthesis requires an H_2/CO ratio between 2 and 3, the elementary analysis of biogenic feedstock already shows that the lack of hydrogen limits carbon conversion. The highest carbon conversion is achieved within MeOH and DME synthesis with 40 % and 39 % respectively. In contrast, FT and SNG only reach 36 % and 32 %. Additionally, carbon is released in the process steps of pretreatment and gas conditioning in the form of CO_2. Neglecting the hydrogen production without carbon capture, the highest specific CO_2 emissions are in the Fischer-Tropsch and SNG cases, with $22\,t_{CO2}\,h^{-1}$ and $24\,t_{CO2}\,h^{-1}$ respectively. While the carbon balance has only the solid biomass feedstock and, if necessary, a small amount of fuel for torrefaction as input, non-negligible portions of the hydrogen balance are provided by adding water in the full water quench. The hydrogen conversion reaches up to 64 % in the pure H_2 production variant. In comparison, the hydrogen conversion efficiency decreases to 26-55 % for the carbon-containing products. However, only hydrogen routes show a negative water balance with a $5\,t_{H2O}\,t^{-1}_{product}$ demand, assuming complete wastewater treatment. Considering the integration into future energy systems, the water balance, greenhouse gas emissions and feedstock availability will be decisive for the application.

As energy and material-based key performance indicators do not necessarily correlate, a combined conclusion regarding the one best process route is not possible. Furthermore, as topics like sector coupling, polygeneration and circular economy are getting more in focus, the actual case-specific boundary conditions will have the biggest impact on whether such plants will be used on a large scale. Therefore, an economic evaluation based on the presented work and subsequent integration of the process concepts into possible overarching energy systems are needed.

Contributions This paper is the result of the common effort of more authors. **Andreas Hanel:** Methodology, Software, Validation, Visualization, Writing – original draft. **Vincent Dieterich:** Methodology, Software, Validation, Writing – original draft. **Sebastian Bastek:** Validation, Visualization, Writing – original draft. **Hartmut Spliethoff:** Funding acquisition, Supervision, Project administration. **Sebastian Fendt:** Conceptualization, Project administration, Supervision.

5.2 Entrained Flow Gasification-based Biomass-to-X Processes: A Techno-Economic Evaluation (Article IV)

The following section serves as a summary of the results of the in section A.4 attached article. The contents of this section were published in:

Vincent Dieterich, Andreas Hanel, Sebastian Bastek, Hartmut Spliethoff, Sebastian Fendt (2024): Entrained flow gasification-based biomass-to-X processes: A techno-economic assessment. In: Energy Convers. Manag. doi:10.1016/j.enconman.2024.118061

Summary This article is dedicated to examining the use of biomass as a carbon and hydrogen feedstock to supplant conventional fossil-derived feedstocks. The methodology involves process simulations, originally taken from **Article III**, and a techno-economic assessment focused explicitly on various biomass-to-x pathways. Therefore, the same six products, ammonia (NH_3), methanol (MeOH), dimethyl ether (DME), Fischer-Tropsch (FT) syncrude, synthetic natural gas (SNG) and hydrogen (H_2), derived from entrained flow gasification of a generic biomass, are considered. The aim is to evaluate the correlations between technical/energetic and economic performance indicators, all based on similar levels of simulation detail and uniform economic boundary conditions.

The comparative analysis shows a clear cost advantage for carbon-based products, which have a potential cost reduction of up to 34 % compared to their hydrogen-based counterparts. While MeOH, DME and SNG range between 280-300 € MWh^{-1}, H_2 and NH_3 settle at 360-410 € MWh^{-1}. This discrepancy is primarily due to the higher energy requirement of hydrogen-based products and the additional step of CO_2 separation in the process. These additional investments account for at least 500.000 € $MW_{installed}^{-1}$. The cost landscape is broken down further, with variable costs proving to be a key component, accounting for around 50 % of total expenditure. The production of high-pressure and high-value syngas occupies a prominent position within fixed capital expenditure, in particular the share of investment costs for entrained-flow gasification and gas conditioning. In detail, the highest shares within the levelised costs of production, using MeOH as an example, are financing and depreciation (23 %), feedstock costs (15 %), maintenance (12 %) and utilities (11 %). The share of energy input via feedstock (biogenic residues) and electricity (part of the utilities) thus covers around 1/4 of the levelised costs. Compared to power-to-x processes, the dependence on variable costs is lower in biomass-to-x processes.

Despite a generalised approach, no single product proves to be the best choice for all the indicators investigated. However, under the given boundary conditions, methanol shows the most promising results in most indicators. It turns out that the carbon conversion efficiency has a more significant influence on the levelised cost of manufacturing than the hydrogen conversion efficiency. This emphasises the advantage of carbon-based products, particularly given the emerging water electrolysis market and the increasing value of sustainable carbon compared to hydrogen. This strategic insight is particularly important for investment decisions in the coming years of the 2020s and 2030s. It will require a deeper examination of the integration of electricity and hydrogen into the biomass-to-x process.

A sensitivity analysis shows the critical impact of plant lifetime, full load hours and feedstock costs

as factors influencing total costs. The balance between alternative feedstocks and the stability and availability of the plant proves to be a crucial factor for the economic viability of the process.

While carbon-based products have immediate advantages, the horizon for hydrogen-based products strongly depends on the long-term system development. Factors such as the demand and costs for CO_2-negative products (CO_2 abatement) and the potential presence of stranded assets could create an environment for developing hydrogen-based products, even based on biogenic residues. Therefore, strategically using biomass-derived products is essential, especially in hard-to-decarbonise sectors such as aviation and the chemical industry. This analysis underlines the complexity of the decision to synthesise fuels and chemicals, which requires a context-aware and differentiated approach within the energy transition.

Contributions This paper is the result of the common effort of more authors. **Vincent Dieterich:** Methodology, Validation, Software, Visualization, Writing – original draft. **Andreas Hanel:** Methodology, Software, Validation, Visualization, Writing – original draft. **Sebastian Bastek:** Validation, Visualization, Writing – original draft. **Hartmut Spliethoff:** Funding acquisition, Supervision, Project administration. **Sebastian Fendt:** Conceptualization, Funding acquisition, Supervision.

6 Process Evaluation using Energy System Optimisation

As shown in chapter 5, techno-economic assessments can be used to compare two or more processes according to technical and economic parameters; the actual operational use case is not part of the results. Therefore, energy system optimisation is often used to discuss possible use cases. However, this approach needs a large set of boundary conditions, which leads to a high level of uncertainty. As discussed in subsection 2.1.3, several ways of uncertainty consideration are possible. This chapter uses a model of the German energy system to discuss the influence of different foresight variants (section 6.1) and the influence of various factors (section 6.2) on the results.

6.1 Evaluation of Sector-Coupled Energy Systems Using Different Foresight Horizons (Article V)

The following section serves as a summary of the results of the in section A.5 attached article. The contents of this section were published in:

Jerry Lambert*, Andreas Hanel*, Sebastian Fendt, Hartmut Spliethoff (2023): Evaluation of sector-coupled energy systems using different foresight horizons. In: Renew. Sust. Energ. Rev. doi:10.1016/j.rser.2023.113562

*Dual-first authorship, both authors contributed equally to this work.

Summary Energy system modelling and analysis are increasingly used in various fields, from political discussions to company investment decisions. One of the most used methods is energy system optimisation. To be able to simulate scenarios that are as close to reality as possible, these models consider more components and variants and thus are getting increasingly complex. However, this leads to increasing computational effort (for example computing time and storage demand), especially when considering high temporal resolutions over extended time periods.

This article discusses the influence of different foresight methods on the optimisation results. In general, three different foresight methods are known: perfect foresight (optimisation of all timesteps at once with full knowledge of the future), myopia incremental (stepwise optimisation of

specific time increments) and myopia with foresight (stepwise optimisation of time increments with additional foresight knowledge). To evaluate the foresight influence, five variants of the foresight methods are studied:

- Perfect foresight
- Myopia incremental (10 a and 20 a increments)
- Myopia with foresight (10 a increments with additional 10 a and 20 a foresight)

and three scenarios:

- Carbon price (CO_2 emission costs)
- Carbon budget (CO_2 emission limits per sector instead of CO_2 costs)
- Price drop of one technology (based on carbon price scenario)

are used. Besides the changing boundary conditions, all other system parameters remain unchanged. The model mimics the German energy system by considering power, heat, mobility and main base chemical demands. Additionally, the direct European neighbouring countries are modelled in a more abstract way.

In summary, it can be shown that myopia incremental has lower computation times than perfect foresight but always shows higher total system costs. On the contrary, myopia with foresight leads to comparable total system costs as the perfect foresight variant but needs longer to solve the problem. However, the memory demand for perfect foresight is by far the highest.

Regarding the optimisation results, by changing the foresight method, only the 10 a increment myopia shows notable differences in the final energy system composition. Nevertheless, depending on the scenario, minor to significant large differences in installed capacities and plant operation during the transitional years can be observed in all myopia variants. Especially the price drop scenario leads to substantial changes between the foresight variants, showing the high sensitivity of optimisation-based models to small changes in specific system parameters. In contrast, using carbon budgets instead of carbon prices limits the solution space and thus leads to more minor deviations between different foresight methods. However, neglecting limitations in computational resources, there is not one right way for choosing the foresight method. It rather depends on the aim of the respective study. If uncertainties in assumptions like price drops or steep changes in demands are to be evaluated, the foresight horizon should be reduced. On the other hand, if a long-term strategy is to be analysed over a long time period, perfect foresight or myopia with foresight should be used (for example Myopia with 10 a foresight).

Contributions This paper is the result of the common effort of more authors. In details, Andreas Hanel and Jerry Lambert both contributed equally to the work. **Jerry Lambert:** Methodology, Conceptualisation, Software, Validation, Visualisation, Writing – original draft. **Andreas Hanel:** Methodology, Conceptualisation, Software, Validation, Visualisation, Writing – original draft. **Sebastian Fendt:** Project administration, Supervision, Writing – review. **Hartmut Spliethoff:** Funding acquisition, Supervision, Project administration, Writing – review.

6.2 Evaluation of Influential Factors on Energy System Optimisation (Article VI)

The following section serves as a summary of the results of the in section A.6 attached article. The content of this section is currently under review and not yet published:

Andreas Hanel, Toni Seibold, Johanna Gebhard, Sebastian Fendt, Hartmut Spliethoff (2024): Evaluation of influential factors on energy system optimisation. In: Energy Convers. Manag. doi:10.1016/j.enconman.2024.119156

Summary As shown in the theory section (2.1.3), there are many ways in which uncertainties can be introduced into the modelling of energy systems. This article deals with the influence of three influencing factors:

- Scenario variation
- Variation of the underlying weather years (incl. all year-dependent input data)
- Sensitivity analysis of individually selected system parameters

These approaches are evaluated separately and are compared according to their impact on the results of energy system optimisation. Therefore, the same energy system model is used in all evaluations besides the mentioned variations. The model framework is described in section 4.5. However, in terms of the sectors and technologies considered and the spatial resolution, the model used here has been expanded compared to **Article V** (a near emission-neutral system). In general, electricity demand in Germany is expected to double compared to today. However, the share of electricity generated in Germany will only increase by 50 %, which will be accompanied by a significant increase in the amount of imported electricity. In contrast, however, the amount of gaseous energy sources (especially H_2) imported is expected to fall compared to today's natural gas imports.

Three different mobility scenarios are considered in the scenario variation case. Concerning the changing base years, the same model is evaluated in each case with the time series based on data from 2017 to 2021. The sensitivity analysis is based on the Morris methodology and considers 23 parameter groups that influence over 70 individual system parameters.

Analysed separately, all three approaches have a significant impact on the results. The composition of the technology park used and the import/export volumes of electricity, hydrogen and other substances show non-negligible changes. Assuming that an inland methanol (MeOH) production must be sustained, constructing biomass-to-methanol plants in some regions of Germany with 2019 weather data is a cost-optimised decision, whereas no methanol plants would be built in the same region based on 2020 weather data. While the basic demand models remain the same in the base year variation, changing mobility scenarios sometimes lead to significantly higher fuel demand. Among other things, this is reflected in the fact that, depending on the scenario, the German methanol market can be supplied completely sustainably in some cases. At the same time, fossil fuel production plants are still required in more conservative scenarios. Broken down to individual system parameters, the sensitivity analysis shows that the costs of renewable technologies, in particular, have a considerable influence on the results of energy system optimisation. The next

biggest influencing factors are the potential for sustainable feedstock materials, such as biomass and residual materials, and the demand for aviation fuels. Although the variations strongly influenced the use of biomass-to-methanol plants in the previous analyses, the costs of such plants show the smallest influence on the overall system in the list of parameters considered. A significantly higher dependency behaviour can be observed for the costs of renewables.

A direct comparison of the three approaches reveals that the magnitude of the influence on the optimisation results, measured in terms of the relative deviation of the total system costs of the base scenario, is very similar in all cases. For example, changing the base year can have the same effect as changing a single strongly influencing system parameter. The same applies to the assumption of the underlying mobility behaviour.

In summary, it is concluded that when using energy system models for the evaluation of novel processes such as biomass-to-methanol plants, the used scenarios, base year and all boundary conditions must be selected carefully.

Contributions This paper is the result of the common effort of more authors. **Andreas Hanel:** Methodology, Conceptualisation, Software, Validation, Visualisation, Writing - original draft. **Antonia Seibold:** Software, Validation, Visualisation, Writing - original draft. **Johanna Gebhard:** Software, Visualisation, Writing - original draft. **Sebastian Fendt:** Project administration, Supervision, Writing - review. **Hartmut Spliethoff:** Funding acquisition, Supervision, Project administration, Writing - review.

7 Discussion and Conclusion

Discussion

When designing a new technology in the field of sector coupling for future energy systems, the first question is whether it is a large-scale centralised plant or a small decentralised plant. In the present case, the choice of a biomass-to-x plant based on entrained-flow gasification, the advantages are due in particular to the large-scale application. This section combines the results of the articles included as well as an overarching discussion and further interpretation. The example of biomass-to-x systems is chosen to discuss the different approaches of technology benchmarking. However, it explicitly does not go into a detailed presentation of the benchmark of a specific system.

First, it is necessary to analyse whether and on what scale plants of this size are required. As a first step, the meta-study on future power plant requirements in Germany presented in section 2.2 (**Articel I**) shows that significant capacities will be required for the secure supply of electricity. It also shows that natural gas will initially be used for this purpose, but that a switch will be made to synthetic energy carriers from the 2040s onwards. Although the public debate shows that H_2 will be a possibility, SNG is not definitively ruled out as an energy carrier. To summarise, this means that there is a need for both large-scale power plants or comparable, flexible systems for significant amounts of flexible power in the electricity grid and large-scale production of synthetic energy carriers. Based on this assumption, it is reasonable to avoid pure single generation for the operation of a biomass-to-x plant. Instead, the meta-study implies that a polygeneration concept, for example the joint supply of flexible power and heat in addition to the synthesis product, could be beneficial to the system and could therefore be a profitable market. For this reason, the following analyses assume that the inner-German market for the supply of basic chemicals remains unchanged and is thus specified as a boundary condition for system analysis.

Since electricity generation from synthesis gas and heat extraction are technologically independent of the selected synthesis, an analysis of the single-generation process is sufficient for a technological comparison of biomass-to-x processes. In section 5.1 (**Article III**) an energetic/technical analysis of six products based on the identical basic process concept is analysed. In purely energetic terms, it is shown that the selective syntheses (MeOH, DME and SNG) are more efficient than the FT synthesis or the pure H_2 generation (with and without carbon capture or subsequent NH_3

synthesis). However, this neglects the usable heat that could be integrated into external industrial applications or district heating networks, for example. In the case of FT, the waste heat amount is particularly high. From the perspective of polygeneration, the local environment in particular must therefore be evaluated for potential heat consumers. Furthermore, significant differences can be identified, particularly in the carbon and hydrogen utilisation rates. Since one motivation for biomass-to-x plants, or the utilisation of biogenic residues and waste, is to establish a circular economy, particular attention should be paid to these parameters. Thus, one parameter that will be of particular interest for the subsequent energy system analysis can be identified: the influence of feedstock availability on the utilisation of biomass-to-x plants.

Consequently, the proof of technological feasibility and the determination of the basic technological and energy performance indicators are followed by the economic evaluation. In section 5.2 (**Article IV**), a techno-economic analysis of the same six biomass-to-x process variants is carried out. Among the influencing factors of interest for further analyses are the feedstock costs, electricity costs and the full load hours of the plant. The major influencing factor of full load hours in particular confirms the concept of polygeneration, in which a flexible alternation of products is only economical with high utilisation of the system. Depending on the current system status, different products can be offered and idling of the system is avoided. In terms of the variable costs, however, it is clear that the techno-economic analysis alone cannot yet conclusively assess the specific costs of the products. Electricity costs in particular have a varying influence depending on the product, as the H_2 production (and therefore also NH_3) requires additional electricity for purification. It can be deduced here that a variation in input material costs should be included in the system analysis and that different scenarios, and therefore different fluctuations in electricity prices, are necessary.

The combination of the findings from the purely energetic/technical analysis and the techno-economic evaluation of the biomass-to-x systems does not allow a final conclusion to be drawn about the most profitable product without a market analysis. However, MeOH can be identified as one of the most favourable. For the following system analysis, a particular focus is therefore placed on MeOH production, which is modelled under the boundary condition of the industry remaining unchanged in Germany.

Before analysing the influence of the system parameters on the use of the biomass-to-x concepts investigated, the methodological influence is evaluated first, using the model framework presented in **Article II**. Here, the variation of different foresight horizons in section 6.1 (**Article V**) shows that the addressed research question must be clarified first. This dissertation primarily relates to the question of whether and how biomass-to-x plants would be used in a near CO_2-neutral system. The short-term phase of the next few years is being neglected. It can therefore be concluded that for a first analysis of the influencing factors the calculation of only one example year is sufficient. This also helps to reduce the computing time, allowing more variations in the boundary conditions to be carried out. Nevertheless, further studies should carry out operational planning under changing boundary conditions. As can be seen in the last years (Covid 19 pandemic and war in Ukraine), unexpected events can lead to extreme changes in assumptions and boundary conditions and thus will influence the plant operation. Here, the use of a myopia approach with short foresight is advisable to be able to evaluate the influences of unexpected events. For the biomass-to-x process, this means that a high degree of flexibility would enable the process to react to short-term changes in boundary conditions. This again favours the concept of polygeneration The analysis based on the scenario with sudden price drops in particular shows that the expected market volume of a new technology depends heavily on the time at which large-scale market maturity becomes known and the rate of price reductions by reaching mass production.

In the final step, the results from **Articles I** to **V** were then used to carry out an influencing factor analysis in section 6.2 (**Article VI**) using an energy system analysis. The choice of influencing factors evaluated was based on changing scenarios, changing base years and a sensitivity analysis with regard to a selection of system parameters. A change in the underlying weather time series alone, and thus the volatility of renewable electricity generation, in some cases results in close to zero demand for biomass-to-x plants from a system perspective. In contrast, in another year the demand is calculated in the order of several GW of installed biomass-to-x capacity. A comparable picture emerges in the scenario variation, in which only the change in societal behaviour regarding the mobility demand heavily influences the chosen technology portfolio. While weather phenomena cannot be influenced and the result can therefore be interpreted primarily as a risk about revenue expectations, the demand for mobility can be influenced externally. For example, political decisions to promote or ban individual technologies can strongly influence the business case of an explicit biomass-to-x plant. The sensitivity analysis can be used to evaluate additional parameters resulting from the techno-economic analysis: in particular the influence of feedstock availability and plant costs. As can already be seen from various other studies, the costs of renewable energies (photovoltaics and wind power) have the greatest influence on the optimisation result, or more precisely the total system costs. Although the use of biomass and biogenic residues is only possible for some of the processes and direct electrification or at least electricity-based energy carriers are available for almost all applications, the feedstock potential can be identified as the next largest influencing factor. This means that a detailed analysis of the influence of changing feedstock materials on process control and outputs should be investigated in a further step. Especially regarding the changing requirements for gas purification and pretreatment.

The results of the respective articles, as well as the broader interpretations and conclusions, can be summarised as follows:

- Large-scale biomass-to-x plants are necessary for future energy systems.
- A polygeneration approach, producing both flexible power and synthetic energy carriers can be beneficial both from a process and from a system perspective.
- Different biomass-to-x products have varying technical and economic advantages depending on the respective local boundary conditions, for example local waste heat utilisation or feedstock availability.
- The system demand for biomass-to-x plants is significantly influenced by external factors like weather and societal behavior, as well as political decisions and unforeseen events.
- Feedstock availability and renewable energy costs are critical factors influencing overall system costs from a macroeconomic perspective.

As the selected scenario is based on a near-climate-neutral point in time, there is still a residual demand for natural gas or methane. The analysis shows that the influence of natural gas costs at the selected point in time is similar to that of the costs for hydrogen. The systemic value of SNG can therefore be categorised as very high, assuming the significantly larger H_2 volume compared to the SNG/natural gas volume. In contrast, the costs of synthesis have a negligible influence. However, this is due to the fact that there are virtually no alternatives on offer and therefore no competition. This must be included in further studies.

This work already shows many methodological indications for the evaluation of new technologies for use in transforming energy systems. Furthermore, influential parameters can be identified from both a process and a system perspective. For a direct comparison of competing technologies, the same level of detailed analysis (meta-study, process model, techno-economic analysis, evaluation of the influencing factors from a system perspective) would first have to be carried out. This means that for a final evaluation, taking into account the results of the entrained-flow gasification-based biomass-t-x study (the present work), the entire analysis process must also be carried out for all possible competing processes. Thus, if the result shows that the influencing variables are independent of the process, a process comparison based solely on process modelling and economic analysis would be sufficient. However, if a shift towards other influencing variables or a different weighting of the individual variables were to emerge, the evaluation process would inevitably have to run analogously, including system optimisation.

Limitations and Outlook

This study presents a methodological approach for evaluating technologies at both process and system level. By adding the energy system analysis, several other influencing variables can already be discussed and their weighting analysed. Nevertheless, it is important to consider the limitations of the analysis at both the process and system levels.

Process Level What has not yet been taken into account in energy system optimisation is that the maximum operating hours and investment costs will change depending on the input material. For example, it can be expected that more contaminated substances will require more maintenance and more expensive gas purification. Consequently, the higher potential of usable input materials, the goal of a circular economy and higher costs compete as well. In addition to the changing input materials, other competing processes should also be included in the system analysis. These include modifications of the gasification-based biomass-to-x concept as well as fundamentally different approaches such as biological processes. The directly associated possibility of reducing synthesis gas conditioning through H_2 admixture or plasma integration should also be investigated. Although individual influencing variables can be transferred to other technologies, this is only significant to a limited extent depending on the similarity.

System Level Today's energy system models are still far from a 1:1 representation of reality. Some parameters are not or only insufficiently taken into account in the present model. This is largely due to the limitations of the available computing capacities and computing times. For example, social aspects such as irrational decisions in private investments and a lack of acceptance of new technologies or changes in personal behaviour are almost completely absent. By considering studies from the social sciences in the definition of scenarios, this perspective should be included in future studies. From the point of view of taking uncertainties into account in energy system analyses, several methodological approaches are already known. Currently, however, computing time limitations are the main reason why these are not used for very large models. For example, the possibility of time series aggregation should be investigated to make these methods usable for large models. Beyond the methodology, the demand side is implemented in a very simplified manner. It is to be expected that the user side, such as industrial parks and individual companies, will also adapt to the new boundary conditions, meaning that conventional demand-side models will no longer be valid. Furthermore, the demand for raw materials for the construction of renewable technologies has not been sufficiently discussed, neither due to their availability nor due to the resulting dependencies. Although initial studies on raw material requirements for the energy transition are available, these are not yet being used on a large scale as an influencing factor in (global) analyses.

Finally, the need for a high level of detail in the modelling has yet to be confirmed. Here it should be investigated whether a reduction in complexity would nevertheless enable sufficiently valid results. This could reduce the time required for the process to such an extent that the application of combined simulative benchmarks of technologies can be used for a large number of technologies.

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List of Abbreviations

CH_4	methane
CO	carbon monoxide
CO_2	carbon dioxide
DAC	direct air capture
DME	dimethyl ether
EE	elementary effects
FT	Fischer-Tropsch
H_2	hydrogen
MeOH	methanol
NH_3	ammonia
SNG	synthetic natural gas
TCS	trade, commerce and services
WGS	water-gas shift

Declaration of Generative AI

During the preparation of this work, the author used 'Grammarly' and 'DeepL' to improve wording, grammar and punctuation. After using this tool/service, the author reviewed and edited the content as needed and takes full responsibility for the content of the publication.

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A Included Publications

A.1 Operation of Conventional Power Plants During the German Energy Transition: A Mini Review

Reference:
Andreas Hanel, Sebastian Fendt, Hartmut Spliethoff (2022): Operation of Conventional Power Plants During the German Energy Transition: a Mini Review. In: Front. Energy Res. 10. doi:10.3389/fenrg.2022.907251.

A.2 Energy System Optimization using (Mixed Integer) Linear Programming

Reference:
Sebastian Miehling*, Andreas Hanel*, Jerry Lambert, Sebastian Fendt, Hartmut Spliethoff (2023): Energy System Optimization using (Mixed Integer) Linear Programming. In: arXiv. doi:10.48550/arXiv.2308.01882.

*Dual-first authorship, both authors contributed equally to this work.

A.3 Entrained Flow Gasification-based Biomass-to-X Processes: An Energetic and Technical Evaluation

Reference:
Andreas Hanel, Vincent Dieterich, Sebastian Bastek, Hartmut Spliethoff, Sebastian Fendt (2022): Entrained flow gasification-based biomass-to-X processes: An energetic and technical evaluation. In: Energy Convers. Manag. doi:10.1016/j.enconman.2022.116424

A.4 Entrained Flow Gasification-based Biomass-to-X Processes: A Techno-Economic Assessment

Reference:
Vincent Dieterich, Andreas Hanel, Sebastian Bastek, Hartmut Spliethoff, Sebastian Fendt (2024): Entrained flow gasification-based biomass-to-X processes: A techno-economic assessment. In: Energy Convers. Manag. doi:10.1016/j.enconman.2024.118061

A.5 Evaluation of Sector-Coupled Energy Systems Using Different Foresight Horizons

Reference:
Jerry Lambert*, Andreas Hanel*, Sebastian Fendt, Hartmut Spliethoff (2023): Evaluation of sector-coupled energy systems using different foresight horizons. In: Renew. Sust. Energ. Rev. doi:10.1016/j.rser.2023.113562

*Dual-first authorship, both authors contributed equally to this work.

A.6 Evaluation of Influential Factors on Energy System Optimisation

Reference:
Andreas Hanel, Toni Seibold, Johanna Gebhard, Sebastian Fendt, Hartmut Spliethoff (2024): Evaluation of influential factors on energy system optimisation. In: Energy Convers. Manag. doi:10.1016/j.enconman.2024.119156