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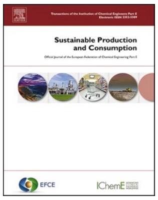

Optimal design of a sector-coupled renewable methanol production amid political goals and expected conflicts: Costs vs. land use

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ABSTRACT

Methanol is an important bulk chemical which can be produced from renewable resources with the currently available technologies and doing so has a high potential for greenhouse gas (GHG) emission reductions for the chemical sector. Reaching the targets for climate change mitigation and biodiversity protection will require designing not only renewable, but also land-efficient chemical production systems. However, under the current economic imperative of cost minimization, the efficient use of land is often not considered during production system design and compromise solutions are left undiscovered, the potential of land-use intensifying technologies stays unknown and the impact of their exclusion, e.g. due to political reasons, is not quantified. This study addresses these issues for renewable production of methanol through the biogas- and power-to-methanol production pathways, which are considered concurrently with processes allowing intensified land use (agrivoltaics, wheat straw anaerobic digestion, heat pumps, wind turbines, etc.) in a previously unexplored technological scope. The designs, as well as the effect of coupling with other production systems (residential heat, electricity, and food) as a strategy to reduce the total annualized costs (TAC) and direct land use, are investigated using the FluxMax approach, an optimization-based design methodology. It simultaneously accounts for the, often neglected, dynamics of renewable energy harvesting, waste-heat utilization and biomass production under the fluctuating renewable resource and product-demand conditions of an example location in Saxony-Anhalt, Germany. Reductions of the TAC of 19 %, direct land use of 9 % and GHG emissions of 12 % for the production system by coupling all four of these products were determined. Furthermore, Pareto fronts were constructed to quantify the trade-off between the conflicting objectives of minimizing TAC and direct land use, demonstrating that land use can be reduced by up to 10 % with minimal extra costs among the available technologies. Political conflicts and goals, which may influence the deployment of the considered technologies, are discussed from a political science perspective and highlight the need for further interdisciplinary collaboration.

1. Introduction

Germany is an example of a developed country working towards the transition to sustainable industrial production, with a high population density and a sharpening conflict for agricultural land. If Germany's goals for this transition, set until the year 2050, are to be met, significant land demand is projected, even extending the total land available for bioenergy production by a factor of 3, leading to dependence on biomass imports (Heinrichs et al., 2021). This suggests a further intensification of the conflicts between food and energy utilization of agricultural land, which have already become more acute due to the widespread development of biogas production for electricity and heat generation (Steinhäußer et al., 2015). Approximately 9800 biogas plants were installed in Germany by the year 2021 (Fachverband Biogas, n.d.). These required about 1.2 million ha for the production of grain crop feedstock, which was around 10 % of the total arable land available in Germany in 2021 (DESTATIS, 2022). However, in contrast to the current use of biogas plants for heat and electricity production, the projections suggest

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that the land available for bioenergy is to be used mainly for renewable fuel production (Heinrichs et al., 2021).

Methanol is one of the prospective renewable fuels (Brynolf et al., 2018; Schemme et al., 2020; Schmidt et al., 2018; Dieterich et al., 2020), but also an important platform chemical for Germany's chemical sector. Today, the production of methanol is an established part of the chemical industry with a global demand of 98 million tons in 2019, yet overwhelmingly produced from fossil feedstock, and accounts for around 10 % of the total CO_2 emissions of the whole chemical sector (0.3 gigatons of CO_2 emitted per year) (Kang et al., 2021). Nevertheless, with the possibility to be produced from renewable resources, its high energy density as a liquid at ambient conditions and its use as a feedstock for the plastic industry (e.g. through methanol-to-olefin processes), it has the potential to be an important molecule not only today, but also for the defossilized industry of the future. In our study, we focus on investigating the design of renewable methanol production systems, useful for both energy and chemical industries, in order to guide their continuing development, with special focus on quantifying their land requirements and the costs for their possible reductions to address the intensifying land use conflict.

To produce methanol renewably, there are two pathways: the biomass-to-methanol pathway, either through biomass gasification or anaerobic digestion producing biogas, and the power-to-methanol pathway, in which renewably generated electricity is used to power the processes of water electrolysis, direct air capture of CO_2 and the methanol synthesis process (Kang et al., 2021). These pathways have different characteristics in terms of production costs, land use and operation. Minimizing the costs and minimizing the land use of these production systems are competing objectives, making the design of cost- and land-efficient processes non-trivial with the many process alternatives implementable in either of these two pathways. This is further complicated by the fact that both pathways should be considered simultaneously in the design, as there are already studies that show the benefits of combining them, which will be discussed below. For the production systems utilizing biomass gasification technologies, the synergies arising from combining these two pathways were shown in several techno-economic studies (Leduc et al., 2010; Ali et al., 2020; Zhang et al., 2020; Hillestad et al., 2018; Hannula, 2015; Hannula, 2016; Poluzzi et al., 2022a; Poluzzi et al., 2022b).

Due to the maturity of the biogas industry in Germany relative to the gasification technologies, and since the focus of the study lies on the efficient utilization of agricultural land, the scope is restricted to the biogas path for utilizing biomass through anaerobic digestion. In this context, Peters et al. (2020) identify methanol as a suitable fuel precursor to be produced at the biogas production site, based on the simplicity of the processing steps and a favorable Gibbs energy analysis. The biogas-based methanol synthesis process was also identified as a promising alternative for jet fuel production in the superstructure optimization work of Kenkel et al. (2022), where power- and biomass- to renewable fuel processes were considered simultaneously.

The alternative production processes for the biogas-based methanol production are presented in a couple of techno-economic analyses. Moioli and Schildhauer (2022a) compare three different routes of producing methanol from biogas, including the power-to-methanol pathway, and show that distributed production of methanol in decentralized smaller-scale plants can be competitive with a centralized production facility supplied with biomethane produced at the biogas plant location, supporting the plant concept studied further in this work. Ghosh et al. (2019) compare three process alternatives for a methanol-only production process, where the biogas is reformed and fully utilized for methanol production, as an alternative to just utilizing the CO_2 waste-stream from biogas, a process route we also include in our design.

However, co-producing methanol with other products (sector coupling) can lead to increased efficiency, which was shown for the biogas-based production system in further studies. Gray et al. (2022) calculate the steady state energy balances of biogas production systems combined with different fuel alternatives, among which the integration of the power-to-methanol process led to a 50 % increase of gross energy generated per hectare per year compared to the biogas-only production, showing significant potential for land use intensification. However, this is not a design study and the costs of the production are not evaluated. On the other hand, Furtado Amaral et al. (2020) take the costs into account in their techno-economic analysis of a biogas-based combined methanol-power-heat production system, where the heat and power is generated from the purge stream and off-gases of the methanol process, limiting the absolute demand coverable by the energy products relative to the methanol production. Furthermore, Baena-Moreno et al. (2020) evaluate a co-production process of biomethane and methanol, also investigating the incentive structure, which could make these processes competitive with the fossil-based alternatives.

Combinations with important end products connected to biogas-based production (residential heating, electricity, or food), however, are not considered in previous studies. It is also worth pointing out that all these biogas-focused studies evaluate the processes only at steady state.

In this work, in contrast, we address the dynamic operation of the power-to-X processes using renewable solar or wind energy. That this needs to be accounted for, is among others called for by Poluzzi et al. (2021). Consideration of the dynamic operation of biogas-based production systems supplied with renewable power could only be found for different energy-carrier molecules. Jürgensen et al. (2014) study the utilization of curtailed energy from wind turbines for biogas upgrading to methane in a dynamically operated system. Furthermore, an ammonia-based energy system is designed under dynamic conditions in the work of Palys et al. (2019), in which the ammonia production supplies the fertilizer needs. In their follow up study, they identify the Pareto front between the net present cost and the total nitrogen loss (Wang et al., 2021). This is also one of the only examples where the design of a chemical production system is combined with food production and a multi-objective optimization study is carried out under dynamic conditions. Land requirements, however, are not incorporated as one of the objective functions. These are accounted for in the study of Ramirez Camargo et al. (2022), where a land-neutral pathway for the expansion of renewable fuel production in Brazil is investigated, in which methanol production from CO_2 waste stream from fermentation and renewable hydrogen is considered in a linear programming optimization-based design approach. The authors show that wind power-based production is the most land-efficient, but a combination of solar and wind power is the cheapest, highlighting the competing objectives of minimizing the production costs and minimizing the land use.

In view of the expected sharpening of the agricultural land use conflict and the goal to defossilize the industry, there is a need to alleviate the demands that the biomass-based production systems impose on the agricultural land. As the current state of the literature suggests, there is deficit for studies incorporating minimization of the land requirements together with the costs early during the design of biogas-based methanol production systems, while considering their inherent dynamic operation. To this end, we investigate the trade-off between the costs and agricultural land use for future renewable production systems with no direct fossil resource use. We utilize a similar methodology as Ramirez Camargo et al. (2022) and Wang et al. (2021) – an optimization-based design with multi-objective optimization to identify cost- and land-efficient, biogas-based production systems for chemicals (methanol), energy (heat and electricity) and food (wheat grain), while considering its dynamic operation. Such sector-coupled production systems are interesting to investigate as the technologies producing the different products overlap, meaning they can also be co-utilized during different periods of dynamic operation saving the total capital expenditure (CAPEX). Additionally, the waste-streams of mass and energy can be interchanged for more efficient combined production. Using actual demand profiles for residential heating and electricity throughout a year, the goal of this study is to quantify the reductions of production costs and land use achievable by sector coupling for a renewable methanol production plant.

The novelty of this work, among others, lies in the extensive set of considered process alternatives, spanning the energy generation, chemical production, biomass production, storage, and utility subsystems. They have been considered simultaneously for the design of the production system, which has been allowed by the used optimization-based design approach. Of special interest are the technologies that intensify land use (utilization of agricultural waste streams – wheat straw for anaerobic digestion; agrivoltaic solar energy generation processes). Additionally, waste-heat utilization technologies (heat pumps, heat engines like organic Rankine cycles and steam turbines), which can also reduce the land demand through increased efficiency (less land intensive biomass and renewable energy generation required), are also included as part of the process network. The effect of the different technologies on the trade-off between costs and land use will be investigated to reach two aims: first, to show how they help in blunting the land use conflict and second, to show how the exclusion of these technologies impacts the possible design space of land-efficient renewable methanol production systems.

Designs of renewable production systems are dependent on the local conditions of renewable resources and, to reach the highest efficiency, should be adjusted to a specific mix of available energy fluxes, mass streams and required product demands tied to a concrete location. Therefore, a specific location in Saxony-Anhalt (Germany) has been selected for the design of the methanol production systems in this study as an example of a favorable region for such a production with significant agricultural output, availability of agricultural waste streams (wheat straw), number of biogas plant installations, and relative proximity to methanol production facilities and therefore already existing supply chains. This example demonstrates existing barriers and potentials for optimizing renewable production systems that may be relevant for similar transition processes with the aim of strengthening renewable carbon cycles under existing or emerging distributional land use-related conflicts. Changes in the political framework pressuring traditional land use concepts can lead to such conflicts. Political aspects are discussed in addition to the considerations from a technological point of view in this paper.

The focus on cost vs. land use optimization for a renewable chemical production was targeted after a detailed policy analysis. During the research process, there was a constant exchange between the involved disciplines (chemical engineering and political science) to adjust the analyses and their directions in an iterative process to new findings. The results of the policy analysis (Section 2) and the modeling study (Sections 3 and 4) are discussed in the discussion Section 5. Final conclusions of this interdisciplinary study are summarized in the conclusions (Section 6).

2. Policy analysis

2.1. Policy analysis method

The present study entails contributions from political science, which are based on a scientific literature research and a policy analysis. The considerations from a political science perspective in this paper are mainly based on the analysis of text documents (Ercan, 2016; Mahoney, 2010; Sadovnik, 2017; Mayring, 2019) and fed into the research design and the final design of the model. Using qualitative methods of policy analysis, recent strategy papers, political decisions and political goals, that are related to renewable methanol production and its regulation, have been analyzed – mainly official policy documents from the European Union and the German national government. Besides, reports from science and industry related to the topics covered in this paper and to political debates in the corresponding fields have been considered (see Supplementary material A). Furthermore, in addition to official information platforms of political, scientific, and industrial organizations on different levels, online media reports have been analyzed in order to identify recent debates that are relevant for the research question discussed in this paper (Neal, 2013; Green Saraisky, 2015; Clarke, 2017; Howland et al., 2006). In the following, the results of the policy analysis are summarized to set the scene for the detailed elaborations on the model calculations for the renewable methanol production system.

2.2. Policy analysis results

2.2.1. Political strategies and goals

In recent years, several non-binding and binding political goals have been defined which serve as an orientation framework for the development of future-oriented and sustainable system designs for chemical production. With our considerations, we tie in with recent political debates, strategy papers and decisions on climate change mitigation, biodiversity protection, nature conservation, and energy and resource transition. All the mentioned topics and policy fields are accompanied by land use claims and therefore plans and activities inevitably are accompanied by land use conflicts. For this reason, land use efficiency is a central building block of the model used and for the scenarios calculated in this paper. Concerning the choice and combination of renewable technology options, there is a wide range of possibilities to choose from. As the political context is crucial for the implementation of an industrial project, we refer to recent developments in the political arena and to political goals and strategies that give a direction for the further development both of the chemical industry and the European economy as a whole.

2.2.1.1. Climate and biodiversity policy. In 2015, the United Nations (UN) defined 17 Sustainable Development Goals (SDGs) for the sustainability transition on a global scale until 2030 (United Nations, 2015a). Climate change mitigation (SDG 13) aims at limiting greenhouse gas emissions to stay below a defined concentration of CO_2 and other greenhouse gases in the atmosphere. For climate change mitigation, the United Nations Framework Convention on Climate Change (UNFCCC) specified a goal in the Paris Agreement as a result of the 2015 United Nations Climate Change Conference (COP21):

> Holding the increase in the global average temperature to well below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C above pre-industrial levels, recognizing that this would significantly reduce the risks and impacts of climate change (United Nations, 2015b)

Recent reports published by the Intergovernmental Panel on Climate Change (IPCC) indicate that it is virtually clear that this goal can only be met with profound transformations. It will not be enough to reduce emissions in business-as-usual scenarios. Emission reductions, the use of Carbon Dioxide Removal (CDR) activities and new fully renewable energy and renewable resource based processes are needed (IPCC, 2018; IPCC, 2021; IPCC, 2022). Against this background, the process network in this study aims at minimizing carbon emissions.

For the field of biodiversity and nature protection, the Convention on Biological Diversity's (CBD) parties to the United Nations Biodiversity Conference (COP15) in Montreal adopted the Kunming-Montreal Global Biodiversity Framework (GBF) in December 2022 (United Nations, 2022). This framework addresses biodiversity loss, ecosystem restoration and the protection of indigenous rights and defines 23 targets to be achieved by 2030. One goal in the framework is to put 30 % of the planet (both land and water) and 30 % of degraded ecosystems under protection by 2030 (30 × 30 or 30 by 30 target, today: land 17 %, marine areas 8 % under protection, according to UNEP) (UNEP, 2022). The EU Biodiversity Strategy for 2030 (EC, 2020a) aims at the protection of nature and the recovery of Europe's biodiversity with a plan containing specific actions and commitments until 2030. It has been developed as a part of the European Green Deal and served as proposal of the EU for the

Global Biodiversity Framework (GBF) in 2022. It aims at establishing a larger network of protected areas in the EU, both on land and at sea, by enlarging existing Natura 2000 areas (today: land 18 %, marine areas 8 % under protection, according to the European Commission) (United Nations, 2022; UNEP, 2022; EC, 2022a). Against this background, among others, the process network in this study aims at minimizing land use.

While the 30 × 30 goals still are a soft instrument and have to be further translated to concrete measures on regional and national levels, there are several political strategies and measures introduced by the European Union (EU) and the German government, which refer to and build on the international goals defined in the Agenda 2030 and the Paris Agreement: the revision of the 2001 EU Strategy for Sustainable Development (EU SDS), aiming at a continuous long-term improvement of quality of life (EP, 2016; EC, 2001), the European Green Deal (EC, 2019), aiming at a climate neutral Europe in 2050 and at greenhouse gas emission reductions of at least 50 % until 2030 compared to 1990 levels, and the 2030 Climate Target Plan (EC, 2020b), aiming to ensure that decisions made in the next years are consistent with the goal of climate neutrality by 2050. This goal has been set out as a binding objective in the European Climate Law in June 2021 (EC, 2021a). There are numerous more specific policy papers that focus on different sectors, resources, technologies, and principles and that incorporated the international goals described above.

2.2.1.2. Renewable energy policy. SDG 7 defines the aim of ensuring access to affordable, reliable, sustainable and modern energy for all (United Nations, 2015a) and finds its equivalents in political measures on the European and national levels. The EU 2030 climate and energy framework (EC, 2023a) defines the following key targets for 2030: at least 40 % cuts in greenhouse gas emissions compared to 1990, at least 32 % share for renewable energy and at least 32.5 % improvement in energy efficiency in the European Union as a whole. The EU published its Clean Energy for all Europeans Package (CEP, a.k.a. Winter Package) as a set of proposals for eight legislative acts in November 2016 (EC, 2023b). The package has been completed in June 2019 and is the fourth package of its kind. It aims at a transition away from fossil resources (defossilization) and towards a carbon neutral economy. With the introduction of the EU Green Deal in summer 2020 (EC, 2019), the targets have been revised and strengthened. The EU Green Deal serves as a vision for the sustainability transition of the EU. It comprises 47 measures that aim at reconciling the targets of climate protection and economic growth instead of regarding them as a contrast. The plan aims at decoupling growth from resource use to meet climate targets.

After the Russian invasion of Ukraine in February 2022, a new plan has been added to European energy policy: The REPowerEU Plan (EC, 2022b). It has been developed in response to disruptions on the global energy market which were caused by the Russian invasion and aims at affordable, secure and sustainable energy for Europeans against the background of the war in Ukraine and its consequences. In contrast to previous political decisions, which strongly supported the use of fossil gas, mainly from Russia, as a less harmful alternative to other fossil energy sources like coal and oil, REPowerEU states the goals of phasing out Russian fossil fuels and accelerating the clean energy transition in Europe. The EU defined the goal to make Europe independent from Russian fossil fuels well before 2030 and announced that it will spur massive investments in renewable energies, as they are the cheapest and cleanest energy available. In the plan, the need for a transition of the industry in general and, more specifically, the need for biogenic alternatives to decarbonize the industry are stressed: “Energy efficiency, fuel substitution, electrification, and an enhanced uptake of renewable hydrogen, biogas and biomethane by industry could save up to 35 bcm of natural gas by 2030 on top of what is foreseen under the Fit for 55 proposals.” (EC, 2022b) Fit for 55 refers to a recent EU climate package (European Council, 2022), which expands the European Union Emissions Trading System (EU ETS) and introduces the Social Climate Fund (EU, 2023; UBA, 2023). The goals of decarbonizing and defossilizing the industry and transforming it to the use of renewable energy, renewable carbon, renewable hydrogen and efficient, coupled and cascaded economic processes is also reflected in more specific strategy papers on European and national level.

The European Union developed a diverse and interlinked system of political measures to support the shift from fossil to renewable energies and already increased the share of renewables significantly in the last decades (EC, 2023a). The goal to become net carbon neutral and replace fossil energies possibly to full extent, however, is rather new (EC, 2019). The future role of nuclear energy is currently still subject of political negotiation processes (Wang et al., 2023; Yue et al., 2022; Nian et al., 2022). Nevertheless, our scenario is based on the assumption that our hypothetical post-fossil renewable methanol production system will use renewable energy sources exclusively. In our system design, we hence incorporate the goal of a fully renewable energy-based methanol production, that does not use fossil resources for energy production and is – concerning direct effects – independent from the availability of fossil raw materials on the world market. Our production system hence does not directly generate greenhouse gas emissions from carbon that was formerly bound in the earth crust (Carus et al., 2020). The renewable energy sources that we include in our considerations are the following:

- Wind energy from wind turbines
- Solar energy from photovoltaics and agrivoltaics
- Bioenergy from primary and residual biomass sources

2.2.1.3. Renewable carbon policy. Worldwide, approximately 50 countries support the idea of transitioning their economies towards bioeconomies (Böcher et al., 2020; EC, 2020c). The concept of bioeconomy is spreading since the early 2010s as an alternative to a fossil-based society (Lanzerath et al., 2022; Thrän and Moesenfechtel, 2022). In the EU, the first bioeconomy strategy has been published in 2012, followed by a revised second version in 2018 (Vogelpohl et al., 2022; EC, 2012; EC, 2018). The second bioeconomy strategy aims at a sustainable, circular bioeconomy with 14 concrete measures that are following three key principles:

1. Strengthen and scale up the bio-based sectors, unlock investments and markets
2. Deploy local bioeconomies rapidly across the whole of Europe
3. Understand the ecological boundaries of the bioeconomy (EC, 2018)

According to the EU, the bioeconomy contributes to addressing the challenges of limited resources, climate change, a growing demand for food, feed and energy, land degradation and ecosystem degradation. The German national government, like several other governments in the EU and worldwide, published national bioeconomy strategies with concepts and goals: After the introduction of a bioeconomy research strategy in 2010 (BMBF, 2010) and a bioeconomy policy strategy in 2014 (BMEL, 2014), Germany published an integrated National Bioeconomy Strategy in early 2020 (BMBF and BMEL, 2020), which aims at a transition towards a sustainable and bio-based economy, at independence of fossil resources such as carbon, oil and natural gas and gearing the industry's resource base towards sustainability.

However, the debates on bioeconomy both at the European and the national level have been accompanied by heated disputes and disagreements concerning the environmental effects of economic biomass use and corresponding support programs. Environmental NGOs, agencies, and authorities criticized the agricultural cultivation of biomass for energy production heavily (Lanzerath et al., 2022; Vogelpohl et al., 2022; Backhouse et al., 2021; Otto et al., 2021). For the case of the European Union's biofuels support policy, indirect land use effects of energy crop cultivation were criticized in the so-called *ILUC* debate, first and foremost referring to deforestation of rainforests for palm oil production in the tropics in Malaysia and Indonesia, but also referring to social aspects like land displacement (Backhouse et al., 2021). In addition, the energetic use of food crops has been criticized strongly after a worldwide hunger crisis in 2007/2008, in the so-called food vs. fuel debate (Vogelpohl et al., 2022).

The use of marginal lands for biomass production is one attempt to address the food, energy, and environment trilemma and to resolve land use conflicts, at least to some extent (Tilman et al., 2009). The role of marginal lands for cultivating energy crops has been discussed in the literature for regions worldwide and there are studies that quantify potential biomass yields on marginalized lands for Germany and other regions in Europe (Mellor et al., 2021; Reinhardt et al., 2022; Gerwin et al., 2018; Wagner et al., 2019). However, biomass production on marginal lands usually requires the cultivation and processing of different kinds of energy crops, like *Miscanthus* or hemp, which have a much lower energy density than maize and hence change the economic efficiency of a production system. Furthermore, actually tapping potentials for biomass production identified in modeling studies can be challenging in the real world due to various kinds of fragmentation, e.g. regarding property structures, responsibilities and physical accessibility, as it has been shown for the use of residual and waste biomass (Baasch, 2021). In our study, we focus on the use of arable land in the selected region in Germany for the cultivation of required crops (maize, wheat).

In Germany, land use conflicts related to bioenergy production and political support programs for energy crop cultivation and use were debated in the context of biogas production from agricultural crops (Beer, 2022). After biogas production had been strongly subsidized by the German government with regulations in the Renewable Energy Act, there has been a heated debate on the *maizification* of landscapes in Germany (*Vermaisung*) and the related biodiversity loss due to monocultures. Similar to the European level, there were discussions about the moral question of burning food products directly and indirectly for energy production, while there is still hunger in the world (Böcher et al., 2020; Vogelpohl et al., 2022; Beer, 2022). High costs and high land use for the production of biogenic raw materials are central critical points in the debate on the energetic and material use of biomass as an alternative to fossil raw materials. Building on these experiences and other debates on conflicts of goals concerning land use, biomass production and biomass use, the newer bioeconomy strategies stress the goal of using residual and waste biomass (e.g. wheat straw, municipal bio-based waste) in efficient coupled processes and in a circular system which integrates different renewable, efficient, economic, and environmentally friendly technology options. With our study, we build on the debates and try to find cost-efficient and land use-efficient system designs with an optimized combination of available technologies.

Both the EU and the German national government have published hydrogen strategies in the year 2020 (BMWi, 2020; EC, 2020d). The EU Hydrogen Strategy comprises 20 key actions. The strategy paper had been adopted in July 2020 and until early 2022, all 20 contained action points had been implemented and delivered. The German government's National Hydrogen Strategy had been published in June 2020 and stresses the relevance of green hydrogen as a key resource for the energy transition and the transformation of the industry. In the strategy paper, the goal of the production of 5 GW of green hydrogen until 2030 has been set, the investment of 7 billion Euro for research in Germany and 2 billion Euro for international cooperations in the hydrogen sector, e.g. with Morocco. These examples show that there are various competing and complementary technology options and political strategies which are building blocks for the transition to a resource efficient and climate friendly chemical production of the near future. In our study, hydrogen technology options are included as they play an important role in the trade-off of land use.

Several years and emissions after the Paris Agreement (United Nations, 2015b), it became clear from reports of the Intergovernmental Panel on Climate Change (IPCC) and hence from the scientific community, that at the beginning of the 2020s it is virtually not realistic anymore to reach this goal by limiting emissions alone. IPCC reports show that Carbon Dioxide Removal (CDR) technologies will most likely be needed in order to reach the goal of the Paris Agreement (IPCC, 2018; IPCC, 2021; IPCC, 2022). These technologies capture carbon from the atmosphere and are also referred to as Negative Emission Technologies (NETs) (Koven et al., 2022; Anderson and Peters, 2016). NETs and their different subtypes are currently discussed in diverse scientific disciplines and new concepts and keywords have developed in this field, such as Carbon Capture and Storage (CCS), Carbon Capture and Use (CCU), Bioenergy with Carbon Capture and Storage (BECCS) and Direct Air Carbon Capture and Storage (DACCS) (Wenzelides and Draxl, 2018; Lehtveer and Emanuelsson, 2021; Bui et al., 2018; Fajardy and Mac Dowell, 2017; Ross, 2022). On the one hand, there is the need to extract carbon from the atmosphere to reduce the concentration of CO_2 as a measure of climate change mitigation. On the other hand, alternative sources for carbon are needed for industrial processes that are based on the material use of carbon for production processes (Carus et al., 2020; vom Berg et al., 2022; Lee, 2019). The focus of this paper lies on the second topic: the use of renewable carbon as a resource for industrial production processes. This issue is particularly relevant for the chemical industry as a whole and the plastics industry as a subfield that processes the carbon molecule for production and value creation (Hasan et al., 2021; Queneau and Han, 2022). In the present study, we look at renewable carbon as a resource for industrial production and do not include NETs in the system design. Regarding renewable carbon, we build on the typology developed by Carus et al. (2020), who distinguish four types of carbon, referring to the sphere of origin:

- Geosphere: not renewable, fossil carbon from fossil raw materials
- Technosphere: renewable carbon obtained from recycling of already existing plastics and other organic chemistry products
- Biosphere: renewable carbon gained from all types of biomass
- Atmosphere (and technosphere): renewable carbon from direct CO_2 utilization (carbon capture and utilization – CCU, also Power-to-X)

Carus et al. hence define three types of renewable carbon, excluding carbon from the geosphere:

> Renewable carbon entails all carbon sources that avoid or substitute the use of any additional fossil carbon from the geosphere. Renewable carbon can come from the biosphere, atmosphere or technosphere – but not from the geosphere. Renewable carbon circulates between biosphere, atmosphere and technosphere, creating a carbon circular economy (Carus et al., 2020).

This definition understands recycled fossil carbon, e.g. plastics recycled from bottles that were originally made from fossil raw materials, as renewable carbon (technosphere). In our system design however, we only consider two types of renewable carbon sources: carbon from the biosphere, which comprises all kinds of biomass and is therefore closely linked to the concept of bioeconomy (Böcher et al., 2020; Thrän and Moesenfechtel, 2022; Vogelpohl et al., 2022; Otto et al., 2021), and carbon from the atmosphere, which is captured with new technological procedures and hence comprises all kinds of air capture technologies (also referred to with the term *artificial photosynthesis*) (Goeppert et al., 2012; Faunce et al., 2013). Following these reflections, the renewable carbon sources considered in the model are the following:

- Renewable carbon from primary and residual biomass (biosphere)
- Renewable carbon from Direct Air Capture (DAC) technologies (atmosphere)

2.2.2. *Summary of political goals and implications for the model*

The presented political activities in the fields of sustainable development, climate change mitigation, biodiversity/nature protection, energy and resource transition show the dynamics and the pressure that political and industrial actors currently are confronted with. The phasing out of fossil resources both for energetic and material use is set as a goal in many of the mentioned political strategies. As technologies for a fossil-free and renewable production of energy, carbon, basic chemicals, materials and products already exist and are available on the market, the question remains open how available technologies, solutions and systems can be optimized – in our case for renewable methanol production, bearing in mind growing and differentiating demands for scarce land resources.

Against the backdrop of the developments and dynamics described above, we derive the following framework conditions for the design of a renewable methanol production facility in our study:

- Goals of climate change mitigation and biodiversity/nature protection are integrated
- Only renewable energy sources and renewable carbon from biosphere and atmosphere are considered as resources for energy and carbon in the methanol production process
- Reconciliation of environmental goals and economic industrial production is aspired
- Use of local resources is preferred in order to decrease import dependencies, transport requirements and the corresponding energy demand, resource use and emissions
- Optimization of costs vs. land use while considering the overall greenhouse gas emission reduction potential
- Consideration of the influence of possible revenues from selling carbon allowance through the European ETS

3. Methods

3.1. Modeling approach

To model the production systems with the inherent fluctuations of the renewable resources, we utilize the extended FluxMax methodology presented in our previous work, where it was used to investigate the design of a power-to-methanol process with an extensive process network and forms the basis of our modeling approach (Svitnič and Sundmacher, 2022). It is an optimization-based design methodology, which simultaneously considers scheduling and waste-heat utilization by discretization of the thermodynamic state space and solving the resulting convex network flow problem.

The network is formed by nodes, which represent chemical substances, utilities (heat or work) and processes. The process nodes model the conversions between the chemical substance and utility nodes and their material, heat and work requirements are modeled by generalized stoichiometry coefficients, which are determined a priori to the optimization problem solution. The production capacity of the process nodes is described by the process extent variable. Based on the generalized stoichiometric coefficients and the process extent variable, one can determine the fluxes of mass, heat and work, which are represented by the edges of the process network.

To capture the dynamic operation of the production system supplied by renewable resources, the time domain is included and discretized. Under an economic objective function, the optimizer determines the nominal process extent for each process (which dictates the required CAPEX) and the process extents in each time increment (which dictate the scheduling of the production). Simultaneously it considers the storage processes buffering the fluctuations of the renewable resources (where the nominal storage capacity and the storage capacity in each time increment are variables to be determined). Operation constraints (ramp limits and minimum operating capacities) are included to model a more realistic dynamic operation of the system.

Based on the optimal values of these variables, the design and operation of the production system is determined from the process alternatives of the chemical process, utility, storage, energy generation subsystems. For details of the modeling approach, the reader is referred to the previous publication (Svitnič and Sundmacher, 2022). In this work, we present its further expansion with the biogas-based pathway and land use calculations needed to investigate the cost vs. land-use trade-off for the renewable methanol production. The full optimization problem formulation and the parameters can be found in Supplementary material B.

3.2. Process network

The full process network, representing the process alternatives considered for the design of the production systems, is shown in Fig. 1 and the selection of the considered processes will be commented in the following subsection.

The production of methanol from CO_2 and H_2O is carried out through the direct CO_2-based methanol synthesis route, which was shown to have less by-product formation compared to the syngas route (yet with a smaller reaction rate) and hence also a simpler purification section (Marlin et al., 2018), making it suitable for a smaller scale, decentralized deployment. These are modeled by the methanol synthesis process (MTD_{syn}), where CO_2 and H_2 are converted to raw methanol (mixture of methanol and water), which is purified to pure methanol in the methanol purification process (MTD_{pur}). The inclusion of direct electrochemical production of methanol into the process network of this study was omitted based on the results of techno-economic analyses showing that it is currently significantly more costly than the chemical synthesis route and still has a relatively low TRL (technology readiness level) (Adnan and Kibria, 2020; Harris et al., 2020), whereas the technologies considered in this study have reached at least the industrial demonstration stage (TRL 7). Full list of TRLs of the individual technologies can be found in Supplementary material B.

Water can be converted to hydrogen in two electrolyzer systems considered, which have distinct energetic requirements: proton-exchange membrane electrolyzer (PEM) with its flexible dynamic operation and solid-oxide electrolyzer (SOEC) with increased efficiency allowed by utilization of waste heat (Carmo et al., 2013). The produced hydrogen can also be used as an energy source by using the fuel cell technologies (PEMFC, SOFC – a reversed operation of the SOEC electrolyzer (Lonis et al., 2019) or hydrogen combustion ($H2_{comb}$). Atmospheric CO_2 can be captured by the DAC process (a modular, low temperature adsorption process is assumed for maximum heat utilization in the system) (Fasihi et al., 2019), which was selected ahead of the high-temperature alternative (Keith et al., 2018), due to the small-scale plant capacity and possibility to utilize waste heat from other processes.

The utility system is modeled, as per the FluxMax approach, with heat utility nodes (noted with a U; each with a discrete temperature level), which facilitate indirect heat integration between the different processes. These can be seen as distinct pressure levels of a steam utility system, for example. Besides the heat utility nodes, we have the work utility node (W), which stands for the electricity supply system.

Connecting these different utility nodes, we have utility processes, which model the possible conversions between the different forms of energy: heat pumps (HP), heat engines (HE), coolers (CL), heat exchange (HX), electric heating (EB). The resulting utility network incorporates many alternative paths through which the required energy can be supplied to the production processes or how the waste-heat from these processes can be utilized and the optimizer can select the optimal one.

The complexity of this task is further increased by the many storage alternatives, which can be considered: thermal energy storage (TES) at different temperature levels (here we consider phase change material alternatives), electricity storage in compressed air energy storage (CAES) or NaS molten salt batteries (NAS), liquid organic hydrogen carried storage (LOHC), compressed gaseous hydrogen storage (CGH2). Further details about the selection and modeling of these processes can be found in our previous work on the design of a power-to-methanol production process (Svitnič and Sundmacher, 2022).

In this work, we extend the power-to-methanol process network by

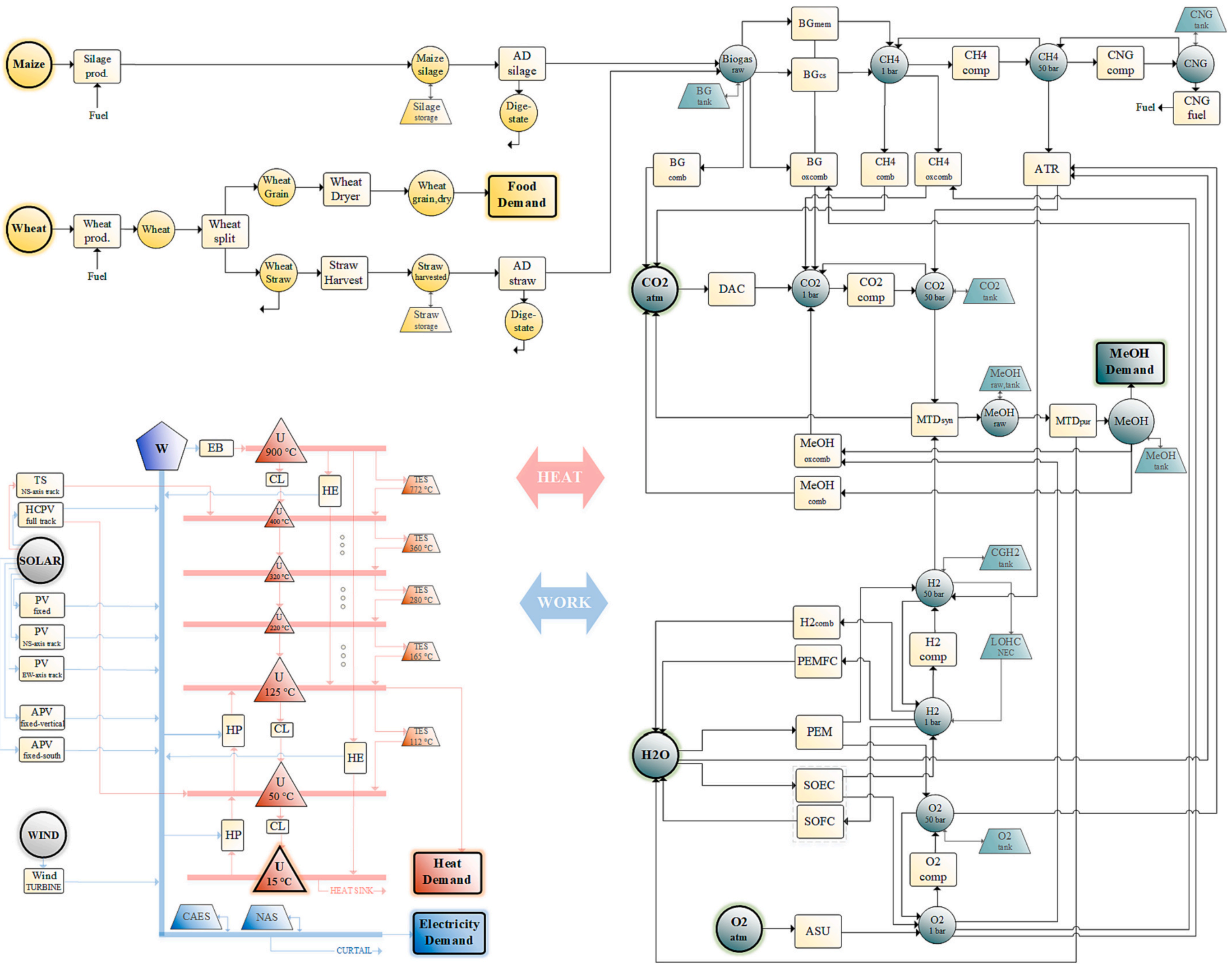

Fig. 1. Process network of biogas-based methanol production including the power-to-methanol pathway, the utility system, biomass production system as well as the options to co-produce food (wheat grain), electricity and residential heating.

including the biomass production/storage processes and biogas processes of the chemical process subsystems. Additionally, the agrivoltaic energy-generation processes are included. In the following subsections, we explain the modeling of these processes.

3.2.1. *Biomass processes*

Two main sources of biomass produced on arable land were chosen to be in the focus of this study: maize silage as the prevalent biomass feedstock for the biogas plants (Daniel-Gromke et al., 2018) and winter wheat as the dominant crop for food production in Germany (Szarka et al., 2021), from which wheat straw can be harvested as an agricultural waste-stream with a high biogas production potential (Dotzauer et al., 2022).

3.2.1.1. Maize and wheat production. Biomass production processes (maize silage and winter wheat) are described in the model by their yield, production costs and fuel consumption (Table 1). The production of the biomass is restricted to particular harvesting periods during the year. These were defined based on the crop calendars (USDA, n.d.) to be a month long period in April for maize planting and September for maize harvesting and October for winter wheat planting and September for winter wheat harvesting. These periods are visualized in the time-series profiles in Fig. 2. As a fully renewable system is designed, the fuel for harvesting cannot be produced from fossil fuels (Paris et al., 2022). We consider that it would be produced in the production system as biomethane used in compressed natural gas (CNG) fueled vehicles, which is an active research topic (Mertins and Wawer, 2022) and such agricultural machinery is already available on the market (Agricultural

Table 1
Yield, production costs and fuel consumption for maize silage and winter wheat production processes. The reported production costs are without the costs for fuel, drying and fertilizer as these are captured in other parts of the model. The fuel requirements of each process are then covered by compressed natural gas (CNG) based on the lower heating value of methane, the breakdown for the fuel demands is shown in Supplementary material B.

	Maize silage	Winter Wheat	Ref.
Yield (t_{DM}/ha)	15.3	11.5	(Zeller et al., 2012)
Production costs (EUR/ha)	1665	931	(Degner, 2019a; Degner, 2019b)
Fuel consumption planting (kWh/(ha a))	1290	1290	(Gerin et al., 2008)
Fuel consumption harvest (kWh/(ha a))	851	851	(Gerin et al., 2008)

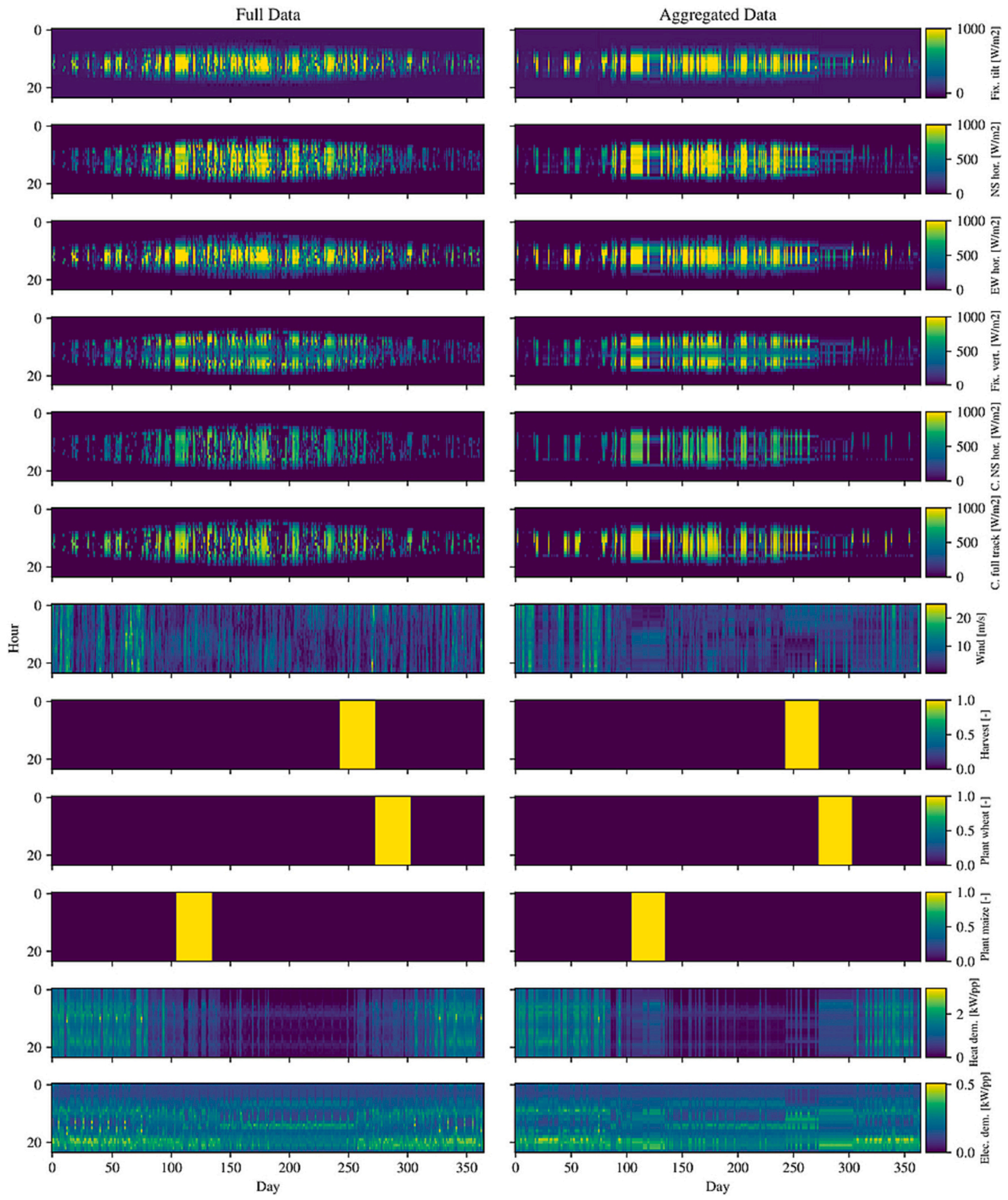

Fig. 2. Renewable resource yearly profile and aggregated data with 24 typical days showing irradiation area hitting aperture area of PV panels with south-facing fixed tilt orientation (Fix. tilt), horizontal (hor.) one-axis tracking with north-south (NS) or east-west (EW) orientation or a fixed vertical (Fix. vert.) agrivoltaic panels. Furthermore, the direct irradiation hitting the aperture area of concentrating parabolic troughs for thermal energy generation with north-south horizontal tracking (C. NS hor.) or highly concentrating photovoltaic panels with two-axis tracking (C. full track) and wind speed at hub height (Wind). The periods where harvesting is carried out (Harvest) and planting of wheat (Plant Wheat) or maize (Plant maize) are also included, as well as residential heating demand (Heat dem.) and residential electricity demand (Elec. dem.) per person.

Tractors, n.d.). The harvested wheat is split into grain and straw streams in the wheat split process (wheat split) based on the harvesting index of 56 % (Zeller et al., 2012).

3.2.1.2. Drying. Wheat grain needs to be dried for long-term storage to a water content of 14 %. We assume a moisture content before drying being equal to 22 %, which would be a comparable moisture reduction of 8 % with a previous similar study (Palys et al., 2019) for maize harvest and falls within the range reported for cereal grain harvest in Chojnacka et al. (2021). Naturally, the moisture content during harvest would vary year to year, but a higher moisture content is assumed in order to design a robust system. To calculate the energy requirements, the heat for drying out 1 kg of H_2O from biomass is taken as 4500 kJ/kg (Chojnacka et al., 2021). The CAPEX for the drying process is assumed to be 199 EUR/kW_{th}, as reported for a belt dryer for digestate drying (with a GBP: EUR conversion ratio taken as 1.17) (Turley et al., 2016) since no CAPEX for grain drying equipment could be found. This assumption may result in high grain dryer CAPEX and consequently increase the calculated food production costs, since Chojnacka et al. (2021) state there are comparatively cheaper dryer alternatives without providing concrete values. However, it will not affect any technological selection in this study, as there is no alternative process for grain drying and it needs to be selected if wheat grain is produced. Recalculated to a dry biomass matter basis, the dryer consumes 1491 kW/(t_{DM}/h) of 80 °C heat and has a CAPEX of 296,512 EUR/(t_{DM}/h).

3.2.1.3. Wheat straw harvest. If wheat straw is to be utilized as a mean to intensify the land use, the wheat straw harvesting process (Straw Harvest) needs to be selected by the optimizer. This process is described by the straw harvesting costs (29.5 EUR/t_{DM}), which is based on values reported in Zeller et al. (2012) for straw harvest without nutrient replacement costs (as they are covered by digestate return) and in Jensen et al. (2017) including also transport costs. Furthermore, it is assumed that 80 % of the totally produced wheat straw can be utilized for anaerobic digestion and the rest stays in the field (as discussed in Brosowski et al. (2020)).

3.2.1.4. Anaerobic digestion. The mesophilic anaerobic digestion process, operating at 38 °C, produces a stream of biogas (assumed to have a composition of 50 % CH_4 and 50 % CO_2 on the molar basis) and digestate as a by-product (Smyth et al., 2009). Further parameters and results for the calculation of the mass/energy streams of the anaerobic digestion processes, as well as the costs are summarized in Table 2 and were largely based on the balances presented in Smyth et al. (2009).

The digestate stream is to be recycled back to the agricultural land for nutrient recovery, where several studies show its suitability to replace mineral fertilizers (Pastorelli et al., 2021; Möller et al., 2010; Robles-Aguilar et al., 2019; Gissén et al., 2014). We assume that the mineral fertilizer requirements are thus reduced to the minimum and their costs are therefore not included in the biomass production costs or the greenhouse gas emissions. The costs/fuel consumption for the digestate return are already included in the maize silage and wheat production processes.

3.2.2. Biogas processes

3.2.2.1. Biogas separation. The produced biogas containing a 50/50 mol % CH_4 and CO_2 is separated into a stream of pure methane and CO_2. Two different separation technologies are considered: chemical scrubbing (BG_{cs}) and membrane separation (BG_{mem}), which have different energy requirements and CAPEX parameters. The chemical scrubbing process requires 140 °C heat (0.55 kWh/(Nm^3_{BG}/h), 0.15 kWh/(Nm^3_{BG}/h) of electricity for the desorption and has a CAPEX of 2250 EUR/(Nm^3_{BG}/h) (Moioli and Schildhauer, 2022b). The membrane process requires only electrical energy (0.3 kWh/(Nm^3_{BG}/h)), but has a higher CAPEX (4000 EUR/(Nm^3_{BG}/h) (Moioli and Schildhauer, 2022b).

3.2.2.2. Reforming process. Since the direct methanol synthesis process requires CO_2 and H_2 feed, among the several alternatives of reforming technologies, we have chosen the autothermal reformer (ATR) with an incorporated water-gas shift reactor, which was shown to have lower energy consumption and higher exergy efficiency compared to a steam methane reforming process as presented in the work of Kim et al. (2021). Based on this study, we have modeled the ATR process in Aspen Plus to calculate the mass and energy requirements (more information can be found in Supplementary material B, which also shows the sensitivity on the overall results of increasing CAPEX and electricity consumption parameters of the ATR process). The reforming is a high-temperature process with the ATR reactor operating at 950 °C and hence we assume that it has limited ramping flexibility (ramping limit parameters can be found in Supplementary material B).

One of the advantages of this system in our application is the possibility to utilize the O_2 by-product stream of the electrolyzers, which is needed for the ATR process to include the option of synergistic operation of the biogas and power-to-methanol pathways. However, if more O_2 stream is needed, an air separation process (ASU) needs to be installed. It is assumed to have an electricity consumption of 3.36 kWh/kmol of O_2 and a CAPEX of 7654 EUR/(kmol/h) (scaled down to a 200 kmol/h production capacity with a scaling factor of 0.65) as estimated based on previously reported data (Berenschot, 2019).

Table 2
Anaerobic digestion (AD) process parameters.

	Maize silage	Wheat straw	Unit	Ref./comment
Biogas (BG) yield				
Organic dry matter content	94 %	87 %	kg_{VS}/ kg_{DM}	(Gerin et al., 2008; Croce et al., 2016)
Methane yield	0.350	0.234	m^3_{CH4}/ kg_{VS}	(Herrmann et al., 2015; Croce et al., 2016)
BG yield per hectare	449.9	92.6	$kmol_{BG}$/ha	
BG yield per ton of dry matter	29.4	18.2	$kmol_{BG}$/ t_{DM}	
Mass balance				
Inlet (dry matter)	1.00	1.00	t_{DM}/h	mass balance basis
Dry matter content	30 %	78 %	t_{DM}/t_{FM}	(de Jonge et al., 2013)
Inlet (fresh matter)	3.33	1.28	t_{FM}/h	
Mass outlet gas	0.65	0.40	t_{gas}/h	
Mass outlet wet digestate	2.69	0.88	$t_{digestate}$/h	
Energy requirement				
Specific heat capacity of biomass	1.4	1.4	kJ/kg_{DM}/K	(Dupont et al., 2014)
Assumed temperature rise	28	28	K	
Assumed heat losses	15 %	15 %	–	
AD macerating	0.23	0.14	kWh_{el}/ $kmol_{BG}$	(Smyth et al., 2009)
AD mixing	2.84	4.59	kWh_{el}/ $kmol_{BG}$	(Smyth et al., 2009)
AD heat demand (40 °C)	3.49	1.30	kWh_{th} / $kmol_{BG}$	(Smyth et al., 2009)
AD costs				
CAPEX per ton of fresh matter	455,520	455,520	EUR/(t_{FM}/ h)	(Jensen et al., 2017)
CAPEX per kmol of BG capacity	51,720	32,147	EUR/ ($kmol_{BG}$/ h)	

3.2.2.3. Combustion. Combustion processes shown in the process network (Fig. 1) model the combustion chambers based on the lower-heating value of the combusted component, from which the energy released is calculated. Heat engine processes can then be selected by the model to convert this high temperature heat energy into electricity. There are also oxy-fuel combustion processes included into the process network, which introduce the possibility to use the oxygen produced in the electrolysis or air separation processes, to produce a stream of pure CO_2 after the combustion, which can be directly used as a feedstock for methanol synthesis.

3.2.2.4. Storage and compression. Storage of biogas and methane can be selected as compressed gas storage at 250 bar. The costs for these processes are taken to be the same as the costs reported for compressed gaseous hydrogen storage on the per mole basis (760 EUR/kmol)

(Niermann et al., 2021). The compression (charging) processes are modeled in Aspen Plus, where energy streams are determined and then recalculated to the corresponding generalized stoichiometric coefficients (Supplementary material B).

3.2.3. Energy-generation processes

3.2.3.1. Solar and wind energy. The solar generation processes are modeled by considering their orientation based on the position of the sun in the sky and the sun-tracking regimes of the different technologies. Furthermore, an efficiency of converting the solar irradiation, which hits the aperture area of the generation technology, is used to calculate the generated electrical energy. The wind turbines are modeled with a linearized wind turbine performance curve describing the conversion of wind velocities to the electrical energy. Detailed modeling of the energy generation processes is described in Svitnič and Sundmacher (2022).

3.2.3.2. Agrivoltaics. The addition we introduce in this work are the agrivoltaic solar energy generation processes, which can be installed on arable land used for biomass production leading to an intensification of the land use. We take two technologies, which should not restrict the harvesting processes of the biomass products: vertical bi-facial photovoltaic panels (facing east and west) with sufficient inter-row spacing (9 m) to allow agricultural machinery to operate between them (Khan et al., 2017; Reker et al., 2022) and a fixed south-facing photovoltaic panels on a rack above the agricultural land in sufficient height (3 m) and inter-row spacing (9 m) to not restrict the agricultural machinery (Horowitz et al., 2020). For both, we consider the models for calculating the actual solar irradiation hitting the aperture area of the photovoltaic panels based on the position of the panel and sun (Supplementary material B). The costs for the agrivoltaic panels were taken as 1.15 $\$/W_{dc}$ for the vertical panels and 1.84 $\$/W_{dc}$ for the racked panels (Horowitz et al., 2020) and the efficiency of the panels is taken as 15 % (same as for the other photovoltaic panels) (Gabrielli et al., 2018).

3.3. Location selection: criteria and available data

The selection of location was done in such a way to select an agriculturally active area in Germany, which also has a significant wheat production, from which the waste-stream of wheat straw could be utilized in the production system. Based on the maps of mobilizable potential of wheat straw utilization presented in Brosowski et al. (2020), we identify an area in the west of Saxony-Anhalt near Ummendorf (Latitude: 52.160 Longitude: 11.176). At this location there is also a weather station (Station 5158 - Ummendorf, n.d.), from which we gather the wind speed data for 10 m height from 2019 through the Climate Data Center (CDC (Climate Data Center), n.d.). We recalculate it to a 100 m hub height assuming a surface roughness of 0.05 m by an approach shown in Decker et al. (2019), with the resulting average wind speed being 6.2 m/s. The solar radiation data (global horizontal irradiation – GHI, direct normal irradiation – DNI and diffuse irradiation DHI) was taken for the same location and year from Sengupta et al. (2018). It was recalculated based on the particular sun-tracking to the profiles of solar irradiation hitting the aperture area. The renewable resource data have a one-year time horizon with an hourly resolution and, together with the time-aggregated data, are shown in Fig. 2.

Time-aggregation of the full renewable and demand profiles into typical days with k-medoids clustering algorithm using the *tsam* package (Kotzur et al., 2018) was employed to arrive at a computationally tractable model instance. This is a simplification of the data, but allows considering the seasonal, daily and hourly fluctuations of the renewable energy and demand fluctuations. It was shown in a previous study comparing the time-aggregation approaches that for a fully renewable energy system that a clustering algorithm with 12 typical days has led to calculation errors of annual costs within 5 % (Kotzur et al., 2018). In Supplementary material B, we show the effect of the time-aggregation on the costs and process selection for our model and pick 24 typical days, as the lowest number of typical days after which the costs are not significantly affected by increasing the number of typical days.

3.4. Demand of methanol, electricity, heat and food

In order to model the production system where electricity, residential heat and food can be co-produced together with methanol, the demand data is needed. The locally aggregated yearly demand profiles for Saxony-Anhalt for the residential use of electricity and heat reported in Priesmann et al. (2021) were used (Fig. 2). The absolute values for these demands are reported in (Table 3). The food (wheat grain) production demand was determined by taking total production of wheat grain in Saxony-Anhalt (Szarka et al., 2021) and dividing it by the number of residents to get a per capital value scaling with the number of residents.

The number of residents for which the demand should be covered by the production system is taken as 100,000. This was determined by making the costs of the production systems producing electricity, heat and food separately comparable to the costs for a 40 kt/year production of methanol, which was chosen as a capacity of smaller scale methanol production plant.

3.5. Economic objective function

Total annual costs (TAC) are taken as the economic cost function to be minimized for the design of the production systems. The total costs as a sum of all the CAPEX costs for all the processes and storages and extra 11 % of the total CAPEX assumed as indirect CAPEX and maintenance costs, together with the costs for producing biomass streams and labor costs are annualized with the interest rate equal to 7 % as described in Svitnič and Sundmacher (2022), as this is also comparable to values used in recent optimization/techno-economic studies of power-to-methanol processes (Decker et al., 2019). Due to a dynamically changing economic environment in terms of inflation and interest rate hikes used to curb it in the recent period, we include a sensitivity analysis of the influence of the interest rate increases on the TAC in Supplementary material B. For designs of production system, which only produce one product, we calculate the levelized costs, by dividing the TAC with the production capacity of the individual product, to get a value comparable with other studies.

3.6. Land use objective function

As a second objective function to be minimized, we consider the direct land use (which would be the area directly covered by the technologies). As an example for wind turbines, this would cover the land required for the turbine itself, as well as roads leading to the wind turbines for maintenance (it would not cover the rest of the area between wind turbines, which can be used for other purposes). Detailed explanation can be found in Denholm et al. (2009). The land requirements for the energy-generation and biomass production processes, which are the only ones considered, as other technologies have a negligible land requirement in comparison (and could even be stacked on top of each other), can be found in Table 4. The land use objective function is then just the sum of the land-requirements of all the energy-generation and biomass production processes.

3.7. Greenhouse gas emission balance

Neither one of the considered production pathways uses fossil-based carbon/energy sources directly, yet there are indirect greenhouse gas (GHG) emissions, which need to be considered. In this work we include a relatively simple GHG emission accounting system as a post-optimization analysis to investigate the effect of the indirect GHG emissions. Additionally, the potential to sell GHG emission allowances is

Table 3
Absolute demand data for the different products of the production system.

Product	Demand per resident		Number of residents	Demand total		Ref.
Electricity	1832	kWh/pp./a	100,000	183	GWh/a	(Priesmann et al., 2021)
Heat	6598	kWh/pp./a	100,000	660	GWh/a	(Priesmann et al., 2021)
Food (wheat grain)	1.3	t_{DM}/pp./a	100,000	130	kt_{DM}/a	(Szarka et al., 2021)
Methanol				40	kt/a	

Table 4
Direct land use (DLU) parameters (maize silage and winter wheat parameters are calculated as reciprocated values of the yields shown in Table 1).

Energy generation/ biomass production process	Process label	DLU	Unit	Ref.
Photovoltaic fixed tilt	PV FIX TILT	2.9	$m^2_{land}/m^2_{aperture}$	(Ong et al., 2013)
Photovoltaic east-west horizontal axis tracking	PV EW HOR	3.4	$m^2_{land}/m^2_{aperture}$	(Ong et al., 2013)
Photovoltaic north-south horizontal axis tracking	PV NS HOR	3.4	$m^2_{land}/m^2_{aperture}$	(Ong et al., 2013)
Parabolic trough: north-south tracking	TS NS HOR	2.5	$m^2_{land}/m^2_{aperture}$	(Ong et al., 2013)
Highly concentrated photovoltaic full-tracking	HCPV FULL TRACK	6.7	$m^2_{land}/m^2_{aperture}$	(Ong et al., 2013)
Onshore wind turbine (3.0 MW)	WIND ONSHORE	10,000	$m^2_{land}/MW_{turbine}$	(Denholm et al., 2009)
Agriphotovoltaic vertical modules	APV VERT FIX	3.7	$m^2_{land}/m^2_{aperture}$	(Horowitz et al., 2020)
Agriphotovoltaic racked modules	APV RACK FIX	5.2	$m^2_{land}/m^2_{aperture}$	(Horowitz et al., 2020)
Maize silage production	Silage prod.	654	m^2_{land}/t_{DM}	
Winter wheat production	Wheat prod.	870	m^2_{land}/t_{DM}	

quantified as an extra revenue stream for the investigated production systems. For this, GHG emission benchmarks of current industrial process alternatives need to be set. Some are defined directly by the European Commission for the emission trading system of the European Union (EU ETS) (EC, 2021b), others however, needed to be established according to common (fossil-based) process alternatives and are summarized in Table 5.

The calculation of the GHG emissions and revenue from selling emissions allowances including the emission factors used for the individual processes are shown in Supplementary material B.

3.8. Resulting optimization problem

The resulting optimization problem is a linear programming problem, which was implemented in GAMS and solved with the CPLEX solver using the barrier algorithm. The multi-objective optimization with the goal to minimize the total annual costs (TAC) or the direct land use (DLU) is implemented with the ε-constraint method where the direct land use is restricted to a maximum limit in the constraints, which is gradually reduced in each optimization problem to generate the Pareto fronts. The full optimization model (GAMS script, input data file and solver setting file) is included in Supplementary material C.

The size of the most-complex optimization problem instance (considering co-production of methanol, food, electricity and heat) was on the order of 250,000 constraints and 700,000 variables. On a computer with the following specification: Intel® Core™ i5-8265U CPU @ 1.60 GHz, 16 GB RAM, the solution time amounted to ca. 18 min for one model instance with 6 threads running in parallel using the barrier algorithm of the CPLEX solver. The algorithm has been chosen after an iterative procedure of adjusting the CPLEX solver settings and led to faster solution compared to the primal or dual simplex algorithms.

4. Results

The result section of the modeling study is structured as follows: firstly, cost-optimal designs of methanol-only and methanol, electricity, heat and food productions and their scheduling are presented to explain the functioning of the identified systems. Secondly, the cost breakdown in terms of total annualized costs (TAC) for the designs is shown together with the effect of sector coupling. Thirdly, the Pareto fronts for competing objective functions of TAC and direct land use are presented and the effect of individual technologies on the Pareto fronts are shown.

4.1. Cost-optimal design and scheduling

4.1.1. Methanol-only production

Fig. 3 shows the selected nominal capacities of the installed processes for a cost-optimal design of methanol production. The main source of energy and material for this design is maize silage, with only relatively small installation of solar and energy generation processes. Maize silage is converted in the anaerobic digestion process (AD_{silage}) into biogas and is purified into biomethane in the chemical scrubbing process (BG_{cs}). Biomethane is then reformed via the autothermal reforming process (ATR) into a stream of H_2 and CO_2. Methanol synthesis (MTD_{syn}) and methanol purification (MTD_{pur}) processes then produce methanol as the only product in this design. Energy supply to these processes is carried out by a system of heat engines (steam turbines), which convert the heat generated in biogas combustion (BG_{comb}) into electricity. We also see an installation of an organic Rankine cycle

Table 5
Greenhouse gas emission benchmark values for the different products used in this study.

Product	Specific emission		Absolute emission		Comment	Ref.
	Benchmark		Benchmark			
Electricity	376	kg_{CO_2eq}/MWh	68.9	kt_{CO_2eq}/a	EU avg. grid emissions[a]	(DEHSt, 2023)
Heat	170	kg_{CO_2eq}/MWh	112.4	kt_{CO_2eq}/a	ETS benchmark (natural gas)	(EC, 2021b)
Food (wheat grain)[b]	185	kg_{CO_2eq} /t_{DM}	24.1	kt_{CO_2eq}/a	Study on wheat prod. in Poland	(Wiśniewski and Kistowski, 2020)
Methanol	94	kg_{CO_2eq}/GJ	74.8	kt_{CO_2eq}/a	Natural gas based production	(Kang et al., 2021)
Total (all 4 products)			280.1	kt_{CO_2eq}/a		

[a] This emission factor also corresponds to the value for electricity production from natural gas emitting 55.8 t CO_2/TJ of primary energy (Juhrich, 2016) with an efficiency of 56 % (combined cycle gas turbine) including a 0.5 % leakage rate of the total converted CH_4 using the GWP_{100} of 28 for converting CH_4 emissions into CO_2eq on mass basis (iea, 2021).

[b] Wheat grain emission factor for full plant was recalculated for grain only with the harvesting index of 56 % (Zeller et al., 2012).

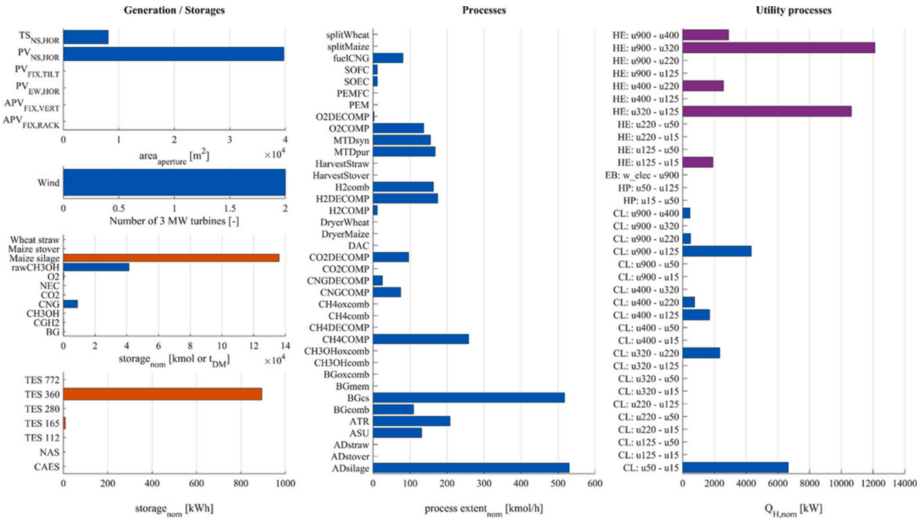

Fig. 3. Design of production of methanol: represented by the installed production capacities (nominal process extents for the chemical processes, nominal hot-stream heat flow $Q_{H,nom}$ for the utility processes). Heat exchanger production capacities are presented in Supplementary material B.

(HE: u125-u15), which converts some of the waste-heat into electricity. No heat pumps are installed, as there is no obvious low-temperature heat demand in the system since DAC has not been selected and residential heating is not produced in the methanol-only production system.

The relatively cheap maize silage storage allows the processes to function stably during the year, as seen in the scheduling profiles in Fig. 4. Maize silage gets stored during the harvesting period and is discharged gradually throughout the year. The other processes adjust their production capacities during the planting and harvesting periods: reduction of production capacities for the methanol synthesis, methanol purification and ATR processes – to reduce the energy demand during this period. Anaerobic digestion and H_2 combustion ($H2_{comb}$) increase their production capacities to cover the fuel (CNG) demands of the harvesting period. The ATR process is regarded as an inflexible process operating at high temperatures, which cannot be so easily ramped up and down, so it keeps operating – generating hydrogen, which gets used as an energy source during the harvesting period.

There are also other processes fluctuating in synchrony with the renewable energy generated in the PV panels and wind turbines to maintain a steady supply of energy. Furthermore, the installation of raw methanol storage (rawCH3OH), allows the methanol synthesis and purification to operate decoupled from each other and shift the methanol purification operation more into the summer period, where there is energy available from the thermal and PV processes. Yet this brings only a limited reduction of the production costs. In our previous work, the flexible operation of the methanol purification process reduced the costs of a power-to-methanol production system up to 2 % (Svitnič and Sundmacher, 2022).

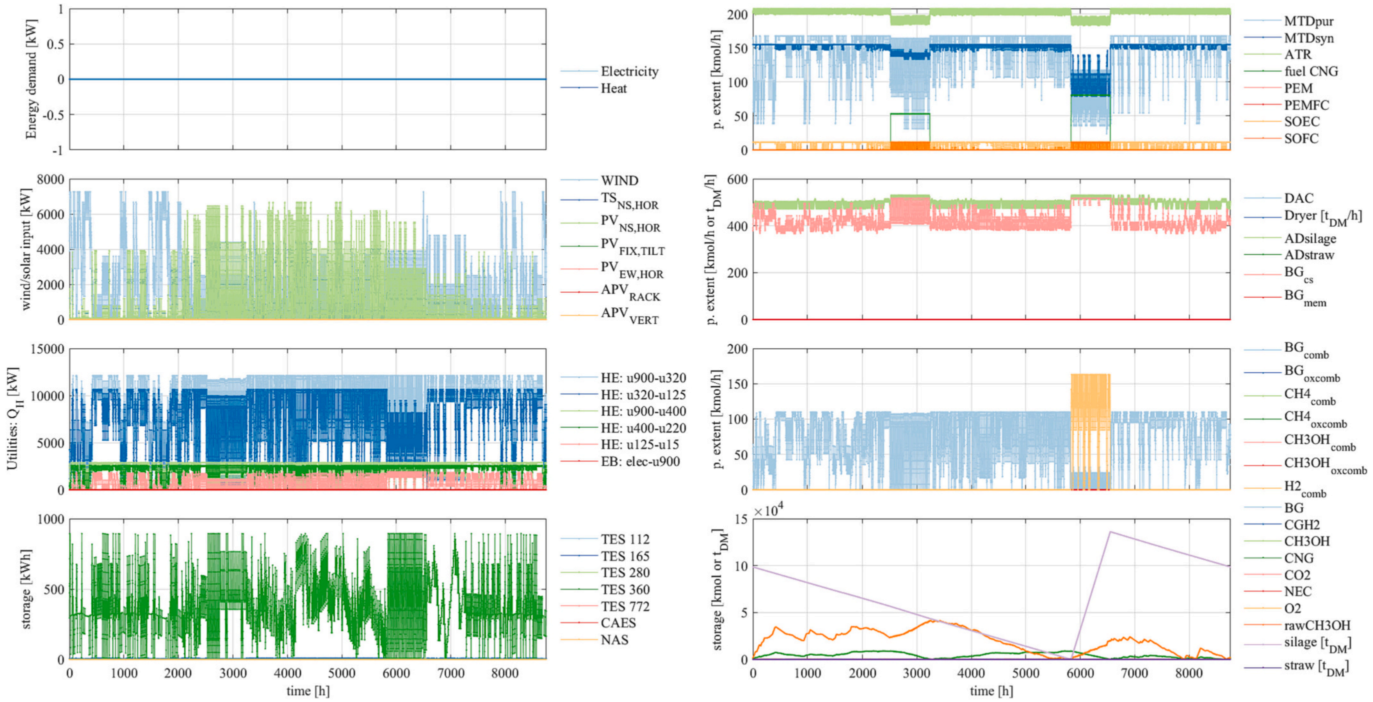

Fig. 4. Scheduling of the operation for cost optimal design with MeOH-only production.

4.1.2. *Methanol, heat, electricity and food production*

For the design of a production system of methanol, residential heating, electricity and food (Fig. 5), a larger proportion of wind power is installed to cover the extra demand for energy, but also a larger capacity for the anaerobic digestion and biogas combustion (BG_{comb}) processes, showing that energy demand is supplied also through the biogas route. ATR and methanol production capacities are also increased compared to the methanol-only production design, showing that methanol also contributes to the energetic needs of producing the other products. Harvesting of wheat straw (HarvestStraw) and its anaerobic digestion (AD_{straw}) are utilized to the full capacity allowed by the wheat production, which is needed to cover the yearly demand of wheat grain.

The energy released in combustion is again converted to electricity in heat engines, yet this time there is no organic Rankine cycle utilizing the excess heat as there is a significant demand for the low-temperature heat for residential needs. A heat pump utilizing waste-heat at 50 °C (HP: u125-u50) is installed as well as a heat pump taking the environmental heat at ambient temperature as the source (HP: u15-u50).

There are also more storage processes installed in significant capacities compared to the methanol-only design. We have the maize silage storage utilized again, but also the wheat straw is stored. Larger storages of raw methanol and methanol are installed and energy is stored in the thermal energy storage processes (TES 360 and TES 165), mainly buffering the daily fluctuations of the supply and demand of renewable energy.

The functioning of the storage processes can be best seen in the scheduling profiles in Fig. 6. The methanol storage is charged throughout the year (as a relatively cheap storage) to cover the large energy demand of wheat grain drying during the harvesting period. In this period, methanol is combusted ($CH3OH_{comb}$) together with H_2 (still produced in the inflexible ATR process during harvesting period).

4.2. *Sector coupling: variants of coupled production*

4.2.1. *Effect of sector coupling on TAC*

In order to determine the sector coupling potential of the future production systems, including electricity, heat, food and methanol production, several production systems with different combinations of these products were designed (Fig. 7).

In all of the production system designs, the biomass resource is the most dominant (maize silage) and only a smaller amount of wind turbines or PV panels are installed as the energy source. Yet, they still feature in these designs showing the complementarity of combining the different energy sources. In the designs with food production (wheat grain), the wheat straw is utilized for anaerobic digestion.

The highest proportion of costs for the storage processes can be seen in the designs for food-only production and methanol + food production. This is due to the fact that for wheat grain drying, the drying heat requirement is relatively large and concentrated to the harvesting period. As not enough energy can be generated during this period (or the installation of larger digesters, reformer, heat engines is not optimal), the relatively cheap methanol storage is installed and methanol is combusted to generate the required energy for the drying process. The proportion of storage is reduced in food productions where electricity and heat are also included, as they provide additional energy sources during the harvesting period, reducing the amount of methanol storage needed to cover the drying demands.

As reference values, we include the production costs where the products are produced separately. These are summarized in Table 6 and show the total annualized costs as well as the levelized costs for the separate products for both the current (2018) and 2030 costs. These are comparable with other levelized costs determined in previous studies for the production of biogas-based electricity and biogas-based methanol production (comparable reference costs for biogas-based heat-only production and fully renewable wheat grain production could not be found). Even the projected methanol production costs in 2030 are higher than the current market price (478 $/t) (Our business, n.d.), showing that such fully renewable production systems are currently not economically competitive with the fossil-based production.

Nevertheless, if two or more products are combined into one production system, reductions brought by synergistic operation were identified. This can be shown by comparing the TAC for the sum of all separate productions and the combined production system. The percent of TAC reductions of a combined production vs. the sum of the separate production of the respective products is included in the top of Fig. 7. It shows that combining electricity + heat, heat + food and electricity + heat + food all bring about reductions above 14 % and up to 20 %. These are all combinations that feature the investment into heat pumps to supply the 125 °C heat to cover the residential heating demand and the drying heat needed to dry grain during harvest. If the installed heat pump is used for both purposes in production systems producing both heat and food, CAPEX savings are achieved.

4.2.2. *Use of methanol as energy carrier in sector-coupled designs*

Interestingly, even in production systems that do not produce methanol as a product, we see the methanol synthesis and purification

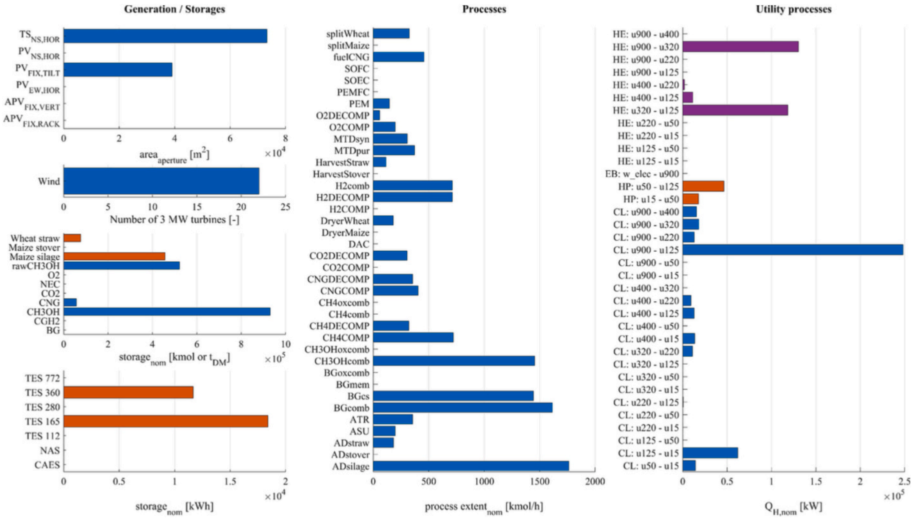

Fig. 5. Design of production of methanol, electricity, heat, food: represented by the installed production capacities (nominal process extents for the chemical processes, nominal hot-stream heat flow $Q_{H,nom}$ for the utility processes). Heat exchanger production capacities are presented in Supplementary material B.

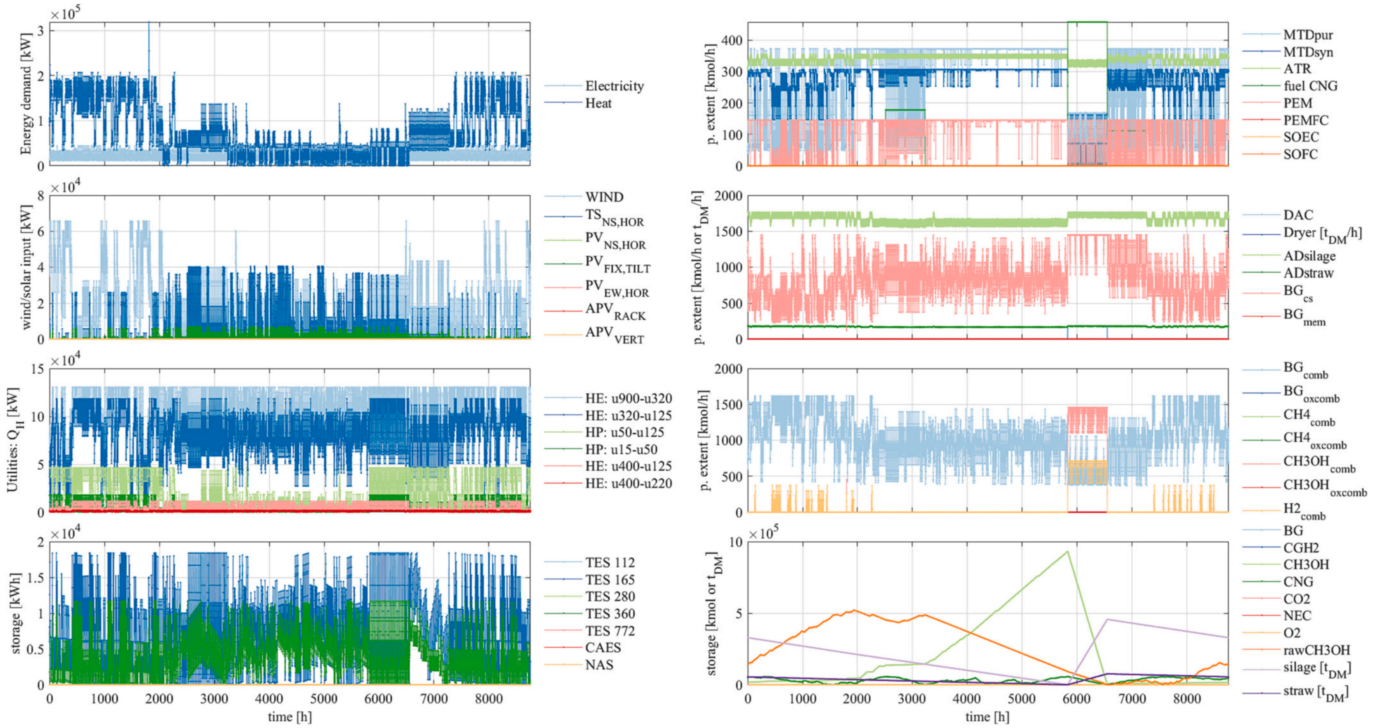

Fig. 6. Scheduling of the operation for cost optimal design with production of MeOH, electricity, heat and food.

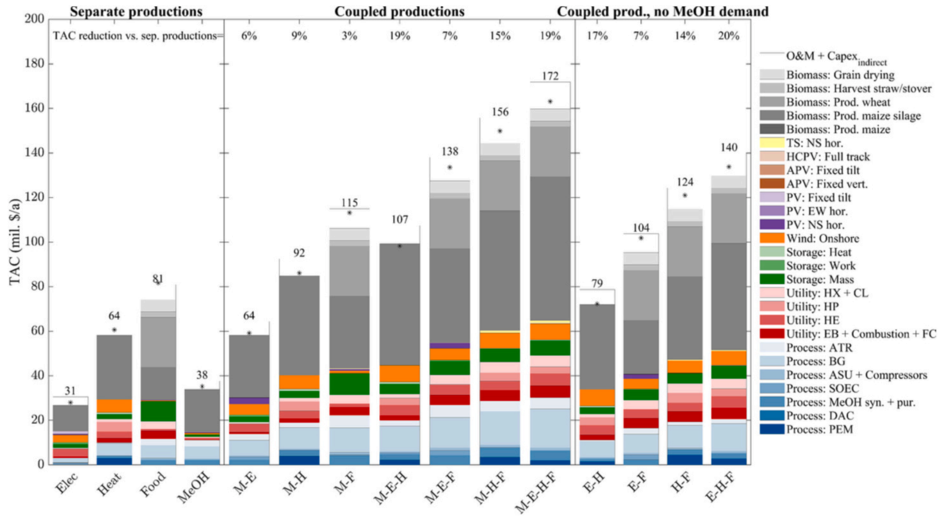

Fig. 7. Total annual costs (TAC) breakdown for production system designs with different product combinations considered (M – methanol, H – heat at 125 °C, E – electricity, F – food (wheat grain)) showing the effect of sector coupling. Percentages on the top refer to TAC reduction of a sector-coupled system vs. the sum of TAC for separate production systems producing the same products. The * marks the total TAC when including the revenue from selling CO_2 allowances with a price of 50 \$/t CO_2eq with a methane leakage rate of 1.85 %.

Table 6
Total annualized and levelized costs for the separate productions of individual products.

Product	Total annualized costs			Levelized costs		Reference costs		Ref.
	Current	2030		Current	2030	Current		
Electricity	30.6	23.8	Mil \$/a	0.17	0.13	0.08–0.17	\$/kWh	(Kost et al., 2021)
Heat	63.9	56.5	Mil \$/a	0.10	0.09		\$/kWh	
Food (wheat grain)	79.9	75.3	Mil \$/a	615	579		\$/t_{DM}	
Methanol	38.1	34.2	Mil \$/a	952	854	455–1013	\$/t	(Kang et al., 2021)

processes being installed. This can be observed most significantly in the food producing systems. In these systems, methanol is used as the energy carrier with its cheap long-term storage providing the best option to shift the energy availability during the year. The energy is then released through a methanol combustion system, supplying the required energy. The significance of this use of methanol is shown in Fig. 8. Here the production systems are designed in the same way as in Fig. 7 with the only difference that the methanol combustion process is excluded from the process network. This prevents the use of methanol as an energy carrier as there is no process to convert methanol into energy.

For these designs, the proportion of storage costs is significantly higher as the more expensive LOHC storage of hydrogen needs to be installed and H_2 is used as the energy carrier to cover the energy demanding harvest period. The percentages of TAC reductions brought by including the methanol combustion process are shown on the top of Fig. 8. These compare the designs in Fig. 7 with the designs in Fig. 8, in which there is no methanol combustion considered.

Even though the inclusion of the methanol production into the combination of products accounted for a relatively small amount of TAC reduction (Fig. 7), it is still a significant part of the combined process for food production with the role of an energy carrier (Fig. 8). The TAC reductions with methanol combustion account for up to 26 % costs reductions (separate food production design). The effect is most significant where the heat production is not part of the production system, as the technologies covering residential heating demand can also be used for supplying the drying process during harvest. Similar utility of methanol for long-term energy storage was also suggested in a recent study (Brown and Hampp, 2023).

When designing the production systems with expected costs for the year 2030, the same behavior can be seen, with slightly lower TAC reduction percentages (Supplementary material B), where a larger proportion of the costs is taken up by wind and solar panels, with their expected reduced future costs.

4.2.3. *Effect of sector coupling on direct land use and GHG emissions*

The effect of sector coupling on direct land use is shown in Fig. 9. Even if for these designs the single objective function is the minimization of the TAC, the direct land use is also reduced by sector coupling by 3–9 %, depending on which productions are coupled together. However, this is not a general conclusion as the total annual costs are often a competing objective with regards to the direct land use of the production. This can be seen in the sector-coupled designs with 2030 cost assumptions (Supplementary material B), where sector coupling for some combinations (electricity + heat) results even in an increase of direct land use. This is because more maize silage production is preferred instead of wind/solar generation technologies, if only a cost-minimizing objective function is incorporated, showing the importance of adding a second objective function for minimizing the direct land use.

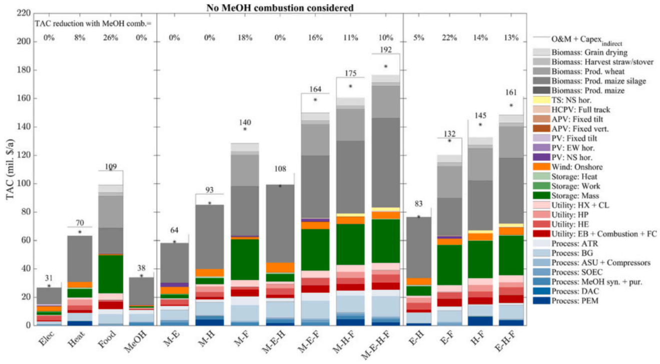

Fig. 8. Total annual costs (TAC) breakdown for production system designs with different product combinations considered (M – methanol, H – heat at 125 °C, E – electricity, F – food (wheat grain)) showing the effect of sector coupling without the use of methanol as an energy carrier. Percentages on the top refer to TAC reductions of a sector-coupled system with methanol used as an energy carrier vs. TAC of a sector-coupled system without methanol use for energy purposes. The * marks the total TAC when including the revenue from selling CO_2 allowances with a price of 50 $/t CO_2eq with a methane leakage rate of 1.85 %.

There is a similarly positive effect of sector-coupling on GHG emission reductions (Fig. 10), with reductions of up to 12 % possible when including all four products. The dominant contributors for these biomass-based designs are the emissions due to methane leakages in the biogas production chain (further analyzed in the later sections of this article) and the emissions due to cultivation of biomass.

4.3. *Multi-objective optimization: TAC vs. direct land use*

In order to study the TAC and direct land use trade-off for the production system designs, we included the direct land use as a second objective function and construct the Pareto fronts presented in the following sub-sections.

4.3.1. *Methanol-only production*

The cost breakdown for the already presented methanol-only production design, which was described in detail, is shown as the rightest bar of the Pareto front in Fig. 11, for which there is almost no investment into PV panels or wind turbines. Since the main source of energy and mass comes from the maize silage production, this production requires a large area of agricultural land (>90 km^2). As the amount of direct land use is restricted (and we move from right to left in the Pareto front), the optimal design starts to shift from maize silage to wind and solar since they have lower direct land use requirements.

In the first portion (>90 km^2), the Pareto-front is flat, showing that roughly 5 % of the direct land use can be saved with almost no cost increase by installing more wind and solar generation technologies to substitute energy generation through biomass.

Yet, already from 90 km^2, the Pareto-front becomes steeper as we start to replace the hydrogen generation (in the most cost-optimal design done fully through reforming of biomethane generated from maize silage). Now also a PEM electrolyzer is installed for H_2 production, making the increase of costs for reducing direct land use steeper. In this way, the increase continues until the design restricted to around 37 km^2.

At this point, the waste-CO_2 stream from the biogas production (left after the separation of biomethane) can no longer cover the CO_2 demand for the methanol production. In the cost-optimal design with no land use restrictions (the most right-hand side bar), the waste CO_2 stream is fully emitted into the atmosphere. As we restrict the land use and more H_2 is produced in the PEM electrolyzer, more of the CO_2 waste stream is utilized to arrive at the desired stoichiometric ratio with H_2 for the methanol synthesis (3 H_2: 1 CO_2). For the 37 km^2 design, the CO_2 in the waste-stream is fully used and a new source of CO_2 needs to be introduced. This is when the DAC process is installed and the Pareto-front becomes steeper again.

In the last section of the Pareto-front (<10 km^2), the land use restrictions are so severe that they do not allow to install any biomass production and even the less land-efficient PV production is replaced by wind turbines, with all the complementarity of the different energy sources being lost and the costs rising extremely.

4.3.2. *Methanol, electricity, heat and food production*

For the combined production of methanol, electricity, heat and food, we see a similar Pareto front as for the methanol-only production (Fig. 12). In this case, the initial flat portion of the Pareto-front (>470 km^2) is even larger and would allow to reduce the land requirements of the production system by >10 % with minimal increase in costs.

The slope of the Pareto front then gradually increases more steeply until the design with around 220 km^2, as the maize silage production is

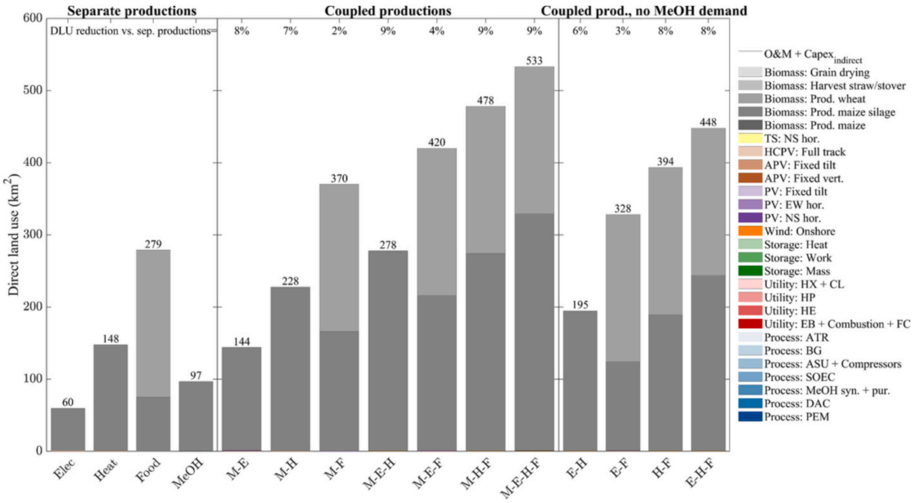

Fig. 9. Effect of sector coupling on direct land use (DLU). Percentages on the top refer to DLU reduction of a sector-coupled system vs. the sum of DLU for separate production systems producing the same products.

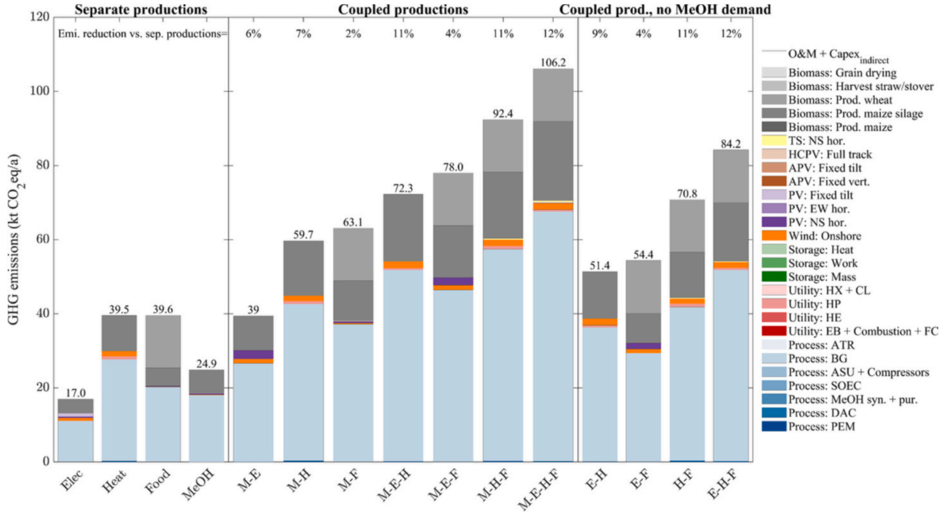

Fig. 10. Effect of sector coupling on the greenhouse gas emissions (GHG). Percentages on the top refer to GHG reduction of a sector-coupled system vs. the sum of GHG for separate production systems producing the same products. The emissions assigned to the biogas process account for methane leakage with a rate of 1.85 % of all produced methane.

replaced with solar and wind energy generation technologies. However, as opposed to the Pareto front for the methanol-only production, there is no DAC being installed, since there is enough CO_2 in the biogas waste-stream (which also originates in the wheat straw harvested as a by-product during the wheat grain production). The proportion of costs for the wheat straw harvest does not decrease as the land use becomes more restricted, which is because the straw is sourced from the same land as the wheat grain and hence calls for no extra land use requirements.

Only for the land use optimal design (most left-hand side bar), we see installation of a small DAC process. The land use cannot be reduced any more for this design (below 200 km^2), since that is the land that is needed to cover the wheat grain demand. Furthermore, for this design, the agrivoltaic technology (vertical PV panels) are included and utilize the land required for wheat grain production even more intensively. Yet, the increase in cost is dramatic, as the wind turbines, which are replaced by the agrivoltaics, are cheaper (and still have a relatively small direct land footprint).

4.3.3. GHG emission sensitivity to methane leakage rates

The GHG emission contributions for the sector-coupled designs have already shown (Fig. 10) that the methane leakage rate can be a dominant, yet highly uncertain, factor in the overall emissions of the studied production systems. In order to quantify its possible impact, we include the sensitivity of the overall GHG emission reduction to the methane leakage rate. In order to use realistic values of methane emissions we refer to a Monte Carlo simulation study based on leakage rate reports from individual processes in the biomethane production chain (Bakkaloglu et al., 2022). Here it was determined that 5 % of the most efficient biogas/biomethane productions simulated had a leakage rate below roughly 1.85 % and that 50 % of the productions had a leakage rate below 5.2 % of the total methane produced (Bakkaloglu et al., 2022). We took the 1.85 % leakage rate as a representative value of an efficiently operated biogas system and used it as a reference in all of the designs of this study except for extra evaluations in this sensitivity analysis.

The results in Table 7 highlight the strong influence of the methane emissions on the possible GHG emission reductions relative to the fossil-based benchmark processes. With a perfect leakage rate of 0 % the biogas pathway could lead to reductions lower than the power-to-

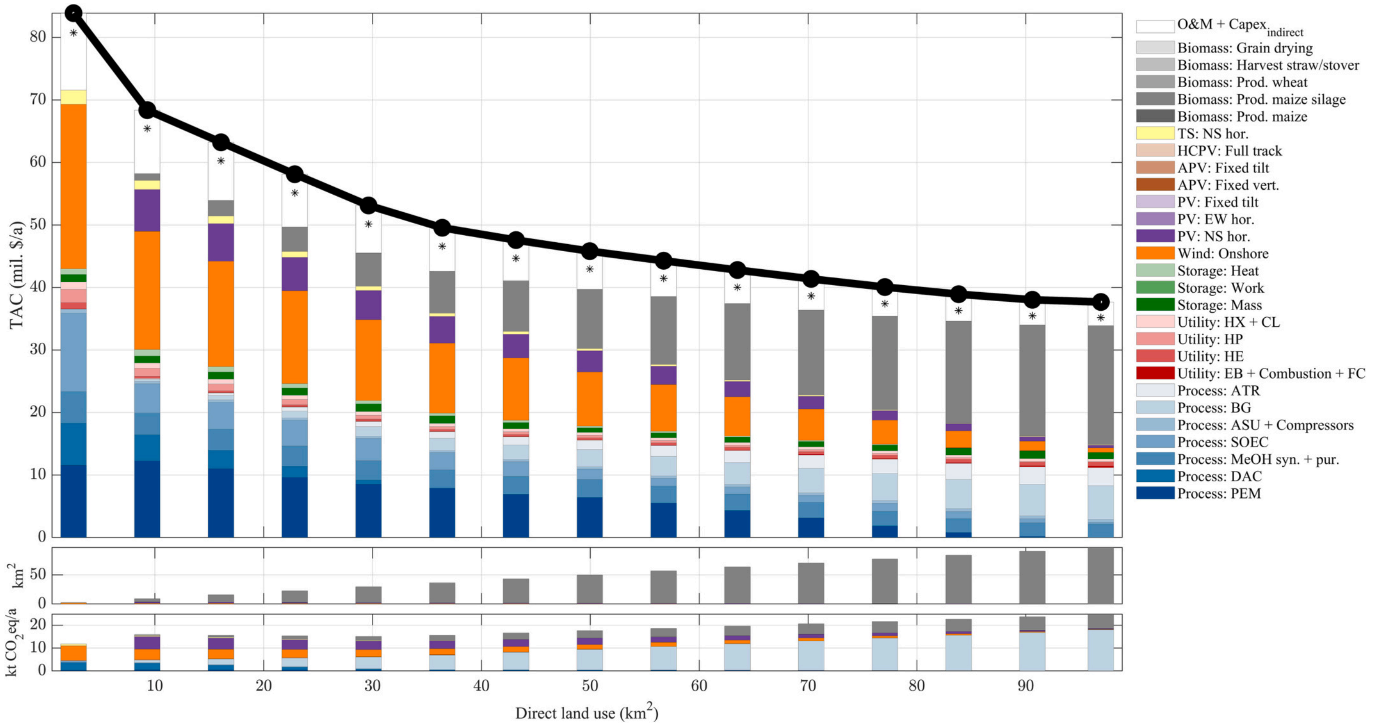

Fig. 11. Pareto front: TAC vs. direct land use (DLU) for MeOH production only with the breakdowns of DLU in km^2 and greenhouse gas emissions in kt CO_2eq/a included in the bottom part. The * marks the total TAC when including the revenue from selling CO_2 allowances with a price of 50 $/t CO_2eq with a methane leakage rate of 1.85 %.

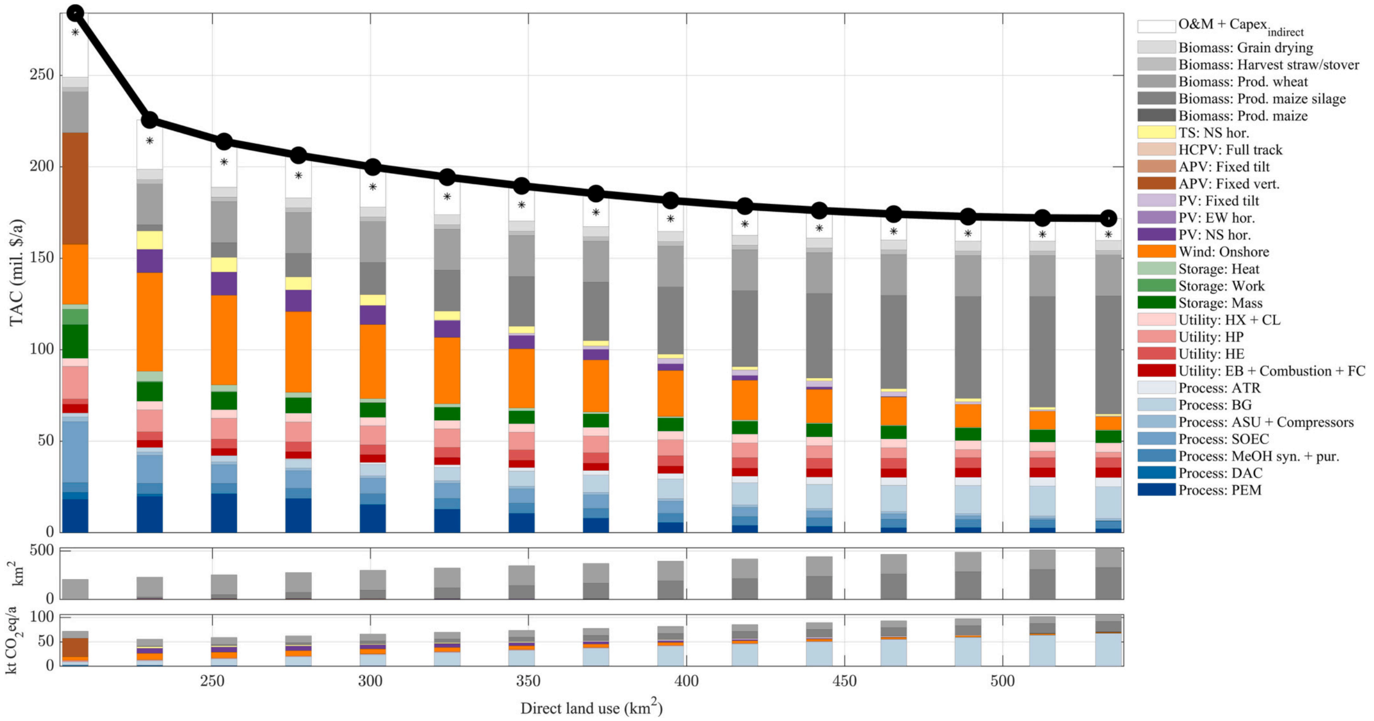

Fig. 12. Pareto front: TAC vs. direct land use (DLU) for MeOH, electricity, heat and food production with the breakdowns of DLU in km^2 and greenhouse gas emissions in kt CO_2eq/a included in the bottom part. The * marks the total TAC when including the revenue from selling CO_2 allowances with a price of 50 $/t CO_2eq with a methane leakage rate of 1.85 %.

methanol pathway. However, even with an optimistic leakage rate of 1.85 % this shifts in favor of the wind/solar based energy production in the power-to-methanol pathway. With common leakage rates of 5 %, only up to one fourth of GHG emissions of the fossil-based process alternatives could be reduced.

4.3.4. Methanol, electricity, heat and food production with no wind energy

The wind turbine technology can enjoy lower levels of public

Table 7
Sensitivity to the methane leakage rate. GHG emission reductions expressed as % of the benchmark value: $GHG_{reduction} = 100\ (1 - E_{total}/E_{benchmark})$.

GHG emission reductions for different designs	CH_4 leakage rate		
	0 %	1.85 %	5 %
MeOH - most land intensive (biomass)	91 %	67 %	26 %
MeOH - most land efficient (PtMeOH)	84 %	84 %	84 %
MeOH + Elec. + Heat + Food - most land intensive (biomass)	86 %	62 %	21 %
MeOH + Elec. + Heat + Food - most land efficient (PtMeOH)	77 %	74 %	71 %

acceptance due to esthetic, ecological or political reasons (Sonnberger and Ruddat, 2017). To show its importance for locations with similar wind and solar renewable resources as for the selected location, we include a Pareto-front where we exclude wind turbines from the process network Fig. 13. This serves as an extreme example of wind turbine technology rejection and shows which consequences for costs and land use this would have.

Even for the most cost-optimal design, we see an increase in direct land use and a slight increase in costs. However, as the land use is more restricted and maize silage production is to be replaced, the solar energy generation technologies are more expensive for similar locations and the Pareto front becomes steeper. For this case, the installation of agri-voltaics appears for design restricted to 320 km^2 or less land use. Similar comparison of Pareto fronts for different process networks are analyzed in the following subsection.

4.3.5. *Comparison of Pareto fronts for different process networks*

In Fig. 14 we compare Pareto fronts of designs, which were created by excluding particular technologies from the overall process network from which the optimizer selects. In this way, the importance of the technology for the design of the production systems can be made apparent.

For the methanol-only production in the 2018 cost scenario, we see the significant effect of excluding wind turbines from the process network. Furthermore, excluding the power-to-methanol pathway (no electrolyzers, no DAC, no solar or wind energy generation technologies) does not allow to reduce the direct land use significantly. Here, the impact of having wind and solar generation technologies as part of the of the cost optimal designs is shown: with the full process network the required land area is 97 km^2 and levelized costs are 952 $/t of methanol. Without the wind and solar generation technologies the cost optimal design (the most right-hand side point of the “No PtMeOH” Pareto front) the production system requires 106 km^2 with levelized costs of 974 $/t of methanol.

It also shows how replacing purely the energetic requirements from maize-silage-based to wind/solar-based has a potential to reduce the land requirements (Pareto front with no electrolyzer vs. the Pareto front for full process network) for a methanol-only production system with current costs. If the costs however reduce more substantially for the wind/solar generation technologies compared to the maize-silage pathway (as in the 2030 costs assumptions), this would no longer be possible as the cost-optimal design would already incorporate an installation of an electrolyzer (and removing it would cause higher costs).

With the 2030 cost assumptions, the power-to-methanol path becomes competitive with the maize-silage path even for the cost-optimal scenarios. However, a combination of these sources is still prevalent in the cost-optimal designs, yet the land use can be reduced by shifting from the biomass-based production to the power-to-methanol pathway with little cost increase. The Pareto front without a DAC process considered shows the point at which the waste-stream of CO_2 from the biogas stream can no longer cover the demand for the production and the costs rise sharply.

For the production system with coupled methanol, electricity, heat and food production the impact of the wheat straw utilization is shown.

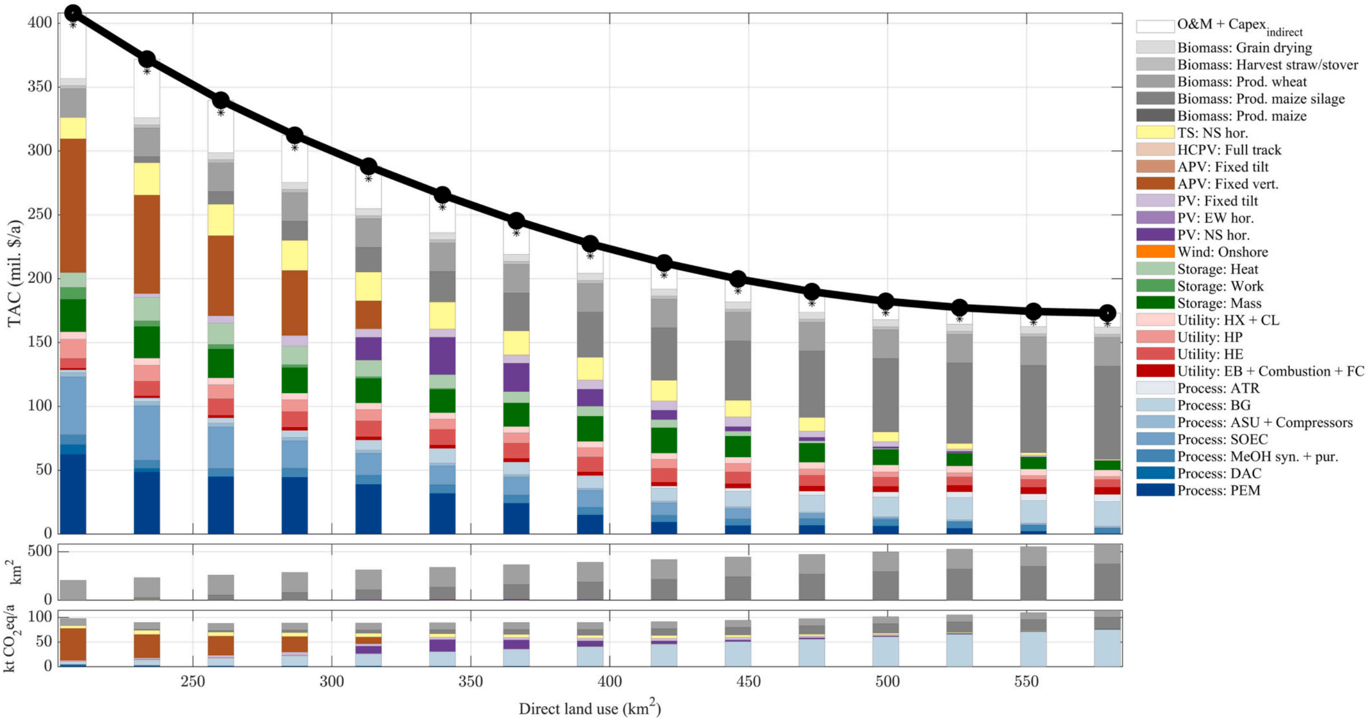

Fig. 13. Pareto front: TAC vs. direct land use (DLU) for MeOH, electricity, heat and food production without any wind energy generation with the breakdowns of DLU in km^2 and greenhouse gas emissions in kt CO_2eq/a included in the bottom part. The * marks the total TAC when including the revenue from selling CO_2 allowances with a price of 50 $/t CO_2eq with a methane leakage rate of 1.85 %.

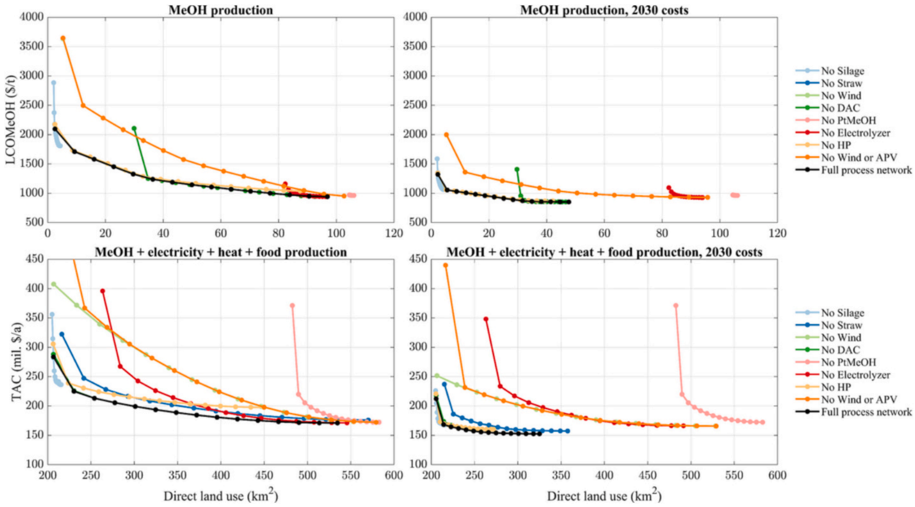

Fig. 14. Comparison of Pareto fronts for different scenarios with 2018 (left) and 2030 (right) cost assumptions, where particular processes were left out of the process network to show their influence for methanol-only (top) and sector coupled production systems (bottom).

Its inclusion can reduce the land requirements of such a production system from 570 to 535 km^2 and the TAC from 176 to 171 mil$/year for the most-cost optimal design (357 to 325 km^2 and 157 to 153 million $/year for the 2030 cost assumptions). Additionally, excluding heat pumps from the production system leads to an increase in costs from 171 to 198 million $/year for the current costs scenario. However, this reduces to a rise from 153 to 164 million $/year for the 2030 cost scenario.

Furthermore, the agrivoltaic PV panels only play a role when the production system is designed under the strictest land use requirements. Up until close to the minimum of land use, the wind turbine is the more efficient technology to produce energy. Only when the limits of land use in the multi-objective optimization procedure start restricting the installation of wind turbines, are agrivoltaic PV panels installed on the area used for wheat grain production. Additionally, even if the power-to-methanol path is excluded from the sector coupled production system, it is important to consider land-requirements as a second objective for the design of the system. The flat portion of the Pareto-front (No PtMeOH) shows that land-requirements can be reduced by adjusting the technological make-up of the production system, with relatively little cost increase.

Reducing GHG emissions and reducing direct land use are for the most part not competing objectives with methane leakage rates of 1.85 % (Fig. 15). For production systems for methanol-only, we see an increase of GHG reductions as we reduce the land requirement, where the CO_2 out of the biogas stream is utilized by installing extra electrolyzer capacity for the additional H_2 needed for the methanol production. When there is no more CO_2 available and the DAC process needs to be installed for further land-reductions, the GHG emissions are no longer reduced, due to the extra energy needed and the associated extra indirect emissions of the energy generation technologies (wind turbines and PV panels). For the most-land restricted designs there is an increase in GHG emission reductions as the PV panels are excluded in favor of the more land-efficient wind turbines, which also have a lower indirect emissions (43 vs. 15 kg CO_2eq/MWh, for a full list of used emission factors and their references see Supplementary material B), however at a cost of losing their compatibility, leading to a sharp increase in costs.

For the sector-coupled designs, the reduction of land-use also leads to a reduction of GHG emissions if wind turbines are not excluded. Only for severely land-restricted designs there is a trade-off between these two objectives as the energy production is shifted from wind turbines towards agrivoltaic PV panels with higher GHG emissions. Please note the sensitivity to the methane emissions presented in figures showing the

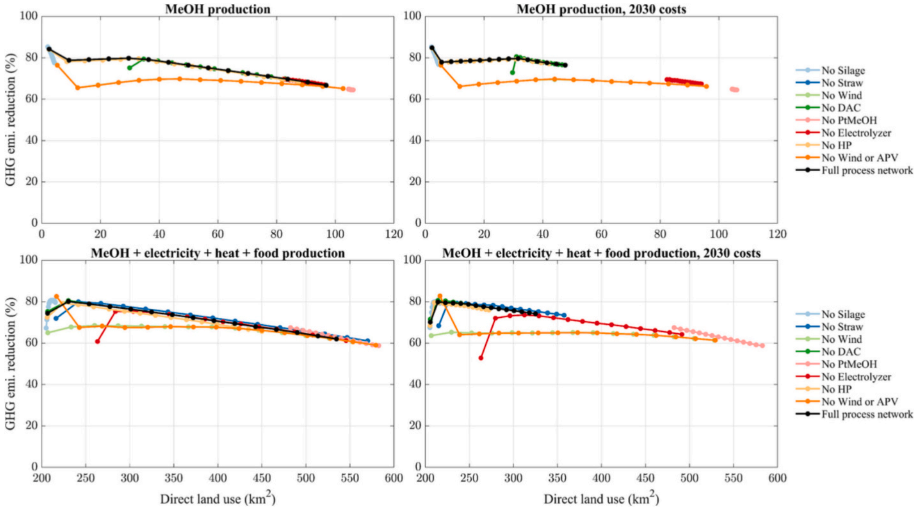

Fig. 15. Greenhouse gas emission (GHG) reductions relative to benchmark processes for different scenarios with 2018 (left) and 2030 (right) cost assumptions, where particular processes were left out of the process network to show their influence for methanol-only (top) and sector coupled production systems (bottom). Corresponds to the designs presented in Fig. 14 with a methane leakage rate of 1.85 %.

relationship between GHG emission and land use reductions for different methane leakage rates, which can be found in Supplementary material B.

5. Discussion

The results of this interdisciplinary study and their implications are discussed in the following along the conceptual framework shown in Fig. 16. First, we discuss possibilities and limitations for technological optimization of renewable methanol production based on the findings of the modeling approach. Second, implications for and interrelations with the political sphere are shown and possibilities for political regulation as well as political costs and risks are discussed (political optimization). Third, we contextualize the findings from the modeling approach regarding the overarching societal goals identified in the policy analysis. The conceptual framework (Fig. 16) summarizes central aspects of this study and serves as an inspiration for future research on both technological and political optimization of industrial production processes against the backdrop of societal goals that aim at the sustainability transition of the economy.

5.1. Technological optimization

In this study, we analyzed how a renewable methanol production plant located at an example location in Saxony-Anhalt Germany can be designed and optimized with a focus on economic costs (TAC) and land use. The model that we developed for this study covers the elements *energy generation*, *utility system*, *storage*, *chemical process*, and *biomass production* in the process network. It allowed calculations for methanol-only production and different kinds of coupled production of food, heat, electricity and chemicals (Fig. 16).

5.1.1. Limitations of the method

The presented results of the technological optimization need to be considered in the context of the modeling approach used and assumptions made. One of the important omissions that the utilized linear model does not allow is to consider the scaling of the investment costs with the installed production capacity. For the majority of the costliest processes (biomass production, wind and solar energy generation, electrolyzers and direct air capture processes – which are all modular in design), the scaling can be considered close to linear due to the numbering up of the production modules. For the chemical processes of methanol production, autothermal reforming and biogas processes, the investment costs were determined at a particular capacity, which fulfills the demand required for the small-scale methanol production of 40 kt/ year. The costs of these processes are small compared to the investment required for the modular processes for energy generation (as shown in the TAC breakdowns), having only relatively smaller impact on the costs (also suggested by the sensitivity to the ATR Capex and electricity consumption parameters in Supplementary material B). It was one goal of this study to capture the breadth of different technological options in a multi-objective optimization approach, which required numerous solutions of the optimization problem with a relatively large superstructure to construct the Pareto-fronts and the sector-coupling product combinations. To do this, a computationally efficient linear programming approach was applied. Adding piecewise linear approximations for the investment costs could be the next step to consider the most-promising identified technological pathways in a more detailed and technologically focused study.

Moreover, the modeling approach assumes perfect foresight, meaning that the renewable energy and the demand profiles over the whole design year are fully known when the optimizer determines the design and scheduling of the processes. The uncertain fluctuations of the wind/ solar energy, yields in harvesting biomass and the demand for the residential electricity and heating are not considered. The model then delivers a design, which would be perfect for the given design year and underestimates the costs related to this uncertainty. Studying the effect of this uncertainty and the role which the complementarity of biogas and the power-to-methanol pathways play in this context would be of further interest. Additionally, the used demand profiles are fixed, based on 2019, so the demand-side response to the changing energy system is not considered. Introducing regulation leading to more energy efficient households or implementing demand side management in the future could influence these profiles and hence the sector-coupled designs identified in this study.

The particular mix of products (methanol, electricity, heat and food) considered in the sector-coupled designs has an influence on the possible location of such a production system. Transport costs have not been considered in this study as we investigated the effect of sector coupling without the transport limitation, to make the design deployable in different decentralized scenarios. Transport of methanol, food and electricity can be done over longer distances supported by existing

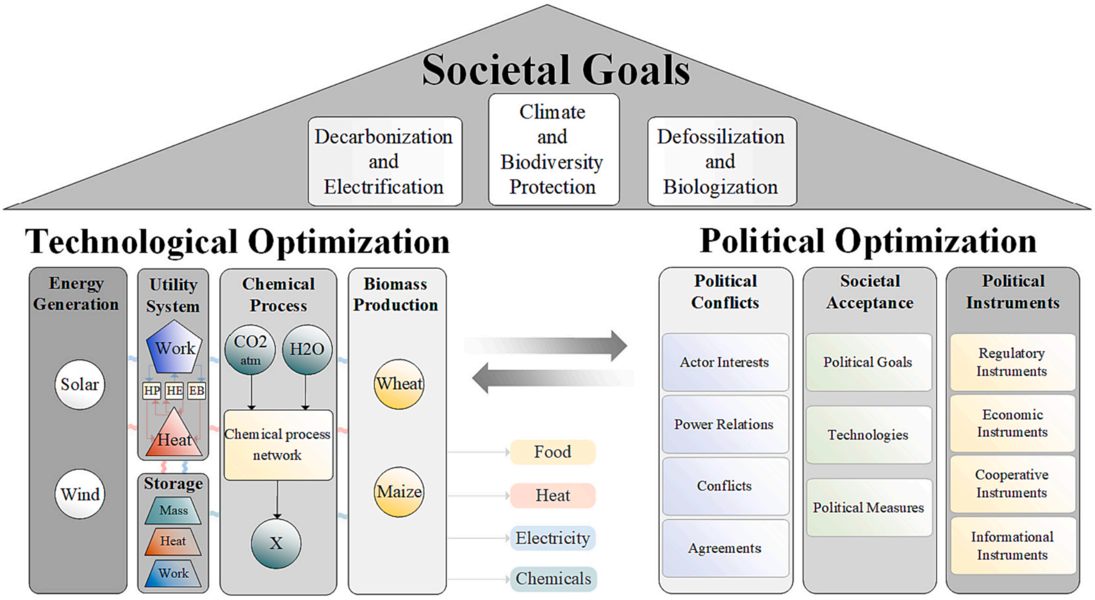

Fig. 16. Conceptual framework for interdisciplinary research on technological optimization, political optimization and societal goals.

infrastructure. However, transporting heat energy over longer distances may be inefficient (Kavvadias and Quoilin, 2018), which would require placing the production system relatively close to the demand location if heat is included as part of the product mix and necessitate additional safety measures and public acceptance. Nonetheless, the reduction of costs for sector-coupled heat production systems determined in this study would suggest that it is worthwhile to investigate this aspect further.

In general, an important part of designing future production systems is the consideration of the impact on water balance. This was not taken into account in our study due to the local environmental conditions of Germany. Here, the agricultural production is predominantly supplied by rainfall and the water requirement for the future energy system of Germany is actually expected to get lower, as suggested in the study of Heinrichs et al. (2021). Nonetheless, under different climate/technological conditions or changes of local climate in the future, the water balance could become an important part of the overall design.

Although the costs for the technologies for the presented early-stage exploratory design could be assumed as identical everywhere, the design of efficient production systems is inherently bound to a certain location with a particular mix of available mass/energy streams and product demand requirements. Therefore, the presented modeling results are best generalizable to locations with similar conditions in terms of: 1) solar and wind energy resource profiles, 2) demand profiles for electricity and heat consumption, 3) agricultural environment, which can support comparable yields of maize silage and wheat. Based on the maize (IPAD, n.d.-a) and wheat (IPAD, n.d.-b) production maps, average solar irradiation (NREL, n.d.) and average wind speed (EEA, 2009) maps for Europe, potential locations, where the identified designs should apply well, are the German states of Saxony-Anhalt, Lower Saxony, North Rhine-Westphalia and Bavaria and the North of France. These regions form a dominant block of wheat production in the European Union (IPAD, n.d.-b) and, under a global consideration, have a similar economic and political environment with the residential heating and electricity profiles also expected to be comparable. Further extrapolation to other agriculturally productive locations in Eastern Europe, North America and China with a similar climate may be inviting, but would need to be investigated in detail, as the local conditions would dictate the concrete design of such a production system.

5.1.2. *Limitations of the scope*

In the broader sense, there are several areas left unexplored, due to the need to limit the scope of this study. We focused on the production of methanol as an important bulk chemical, but there are other interesting molecules, which could be produced in such a biogas-based production system. Ammonia would be a fitting candidate (again a crucial bulk chemical and a potential renewable fuel), which could also function as a direct source of fertilizer for the agricultural production.

One promising technology, which in particular locations could have changed the design identified in this study, is the utilization of salt caverns for gas storage (Caglayan et al., 2020). We have considered a design independent of salt cavern locations in order to identify a geographically more deployable design. Yet, there may be a local geographical overlap, which could allow using salt caverns as a cheaper option for gas storage, possibly altering the identified design.

Furthermore, we consider the use of CNG as the renewable fuel for the agricultural machinery due the low amount of processing steps needed for its production compared to other alternatives and its availability on the market. Methanol, dimethyl ether as a diesel-like replacement or synthetic diesel produced through the Fischer-Tropsch or methanol routes are potential options, but a more detailed study would be needed to select among these alternatives.

Finally, we restricted ourselves to currently the most prominent biogas feedstock (maize silage) and the most abundant food-production related agricultural waste (wheat straw) in the German conditions. However, other biomass sources can be considered for biogas production such as other grain straws, grassland biomass as one of the most plentiful utilizable biogas sources, municipal waste streams (Dotzauer et al., 2022) and other energy crops for biogas production with digestate return (hemp, sugar beet, ley) (Gissén et al., 2014). Potential utilization of waste from animal-based production would need to be evaluated carefully under the consideration of agricultural land use minimization. The land needed for feed production should be taken into account, since shifting to direct food production could lead to significant reductions of land use (Shepon et al., 2018), which could make the dependence on these waste streams unsustainable.

5.1.3. *Modeling results discussion*

Bearing in mind the aforementioned limitations, the results of the multi-objective optimization-based designs are worthwhile to discuss. Taking the purely biogas-based design as the reference and considering an extreme case of market penetration where 100 % of Germany's methanol production of 1.4 mil. t/a (Felkl, 2023) would be produced in such a production system, 35 of them with the assumed 40 kt/a would be required. A combined 3710 km^2 would need to be allocated for this chemical production, which represent ca. 3.2 % of the total arable land of Germany (statista, n.d.) and would add to the 10 % already dedicated to supplying biogas production as of 2021 (DESTATIS, 2022), going against the biodiversity protection goals and leading to further conflict for agricultural land if the current use of biogas would not be repurposed to chemical production.

The trade-off that needs to be made, if direct land use and GHG emissions are to be reduced, is summarized for a selection of designs identified for methanol-only production in Table 8, which suggests that the increase in costs depends on the extent of land-use reductions. As the low-hanging fruit, for the 2018 cost scenario, a 14 % land-use reduction

Table 8

Summary of borderline designs identified for methanol-only production systems with evaluated ratios of production costs, direct land use (DLU) and greenhouse gas emissions (GHG) increases/reductions relative to the reference process of purely biogas-based methanol-only production design. The methane leakage rate in the biogas pathway is taken as 1.85 %.

Methanol-only production system design	Cost scenario 2018			Cost scenario 2030		
	Cost %	DLU %	GHG %	Cost %	DLU %	GHG %
No PtMeOH (purely biogas-based) = reference	964 \$/t	106 km^2	27 kt_{CO2eq}/a[a]	964 \$/t	106 km^2	27 kt_{CO2eq}/a[a]
Full process network (biogas-based, wind + PV)[b]	−1 %	−14 %	−11 %			
Full process network (biogas-based, full CO_2 use)	22 %	−66 %	−41 %	−10 %	−70 %	−43 %
No Silage (power-to-MeOH-based)	47 %	−96 %	−37 %	10 %	−96 %	−35 %
No Silage (power-to-MeOH-based, minimum land)	67 %	−98 %	−59 %	39 %	−98 %	−59 %

[a] Please note that this value already represents a 65 % GHG emission reduction versus the benchmark natural gas based process (75 kt_{CO2eq}/a).

[b] For the 2030 cost scenario, the cost-optimal design for the full process network already contains a PEM electrolyzer utilizing the CO_2 waste-stream, so just a biogas-based design with only wind turbines and PV panels is not identified as in the 2018 cost scenario.

relative to the pure biogas-based methanol production could be achieved by installation of wind turbines and PV panels to supply the electricity needed in the chemical production systems, instead of sourcing it from biogas combustion (possible without an increase in costs as doing so is also the cost-optimal solution). By utilizing the CO_2 waste stream through the use of a PEM electrolyzer in order to reach the stoichiometric ratio of H_2 and CO_2 needed for the methanol synthesis, the land-use can be reduced by 66 %, yet at an increase in costs of 22 %. To gain a further 30 % of land-use reductions, the process would need to be fully based on the power-to-methanol pathway with an overall 47 % increase in costs. In the 2030 cost scenario, the cost-optimal solution shifts towards a combined biogas + power-to-methanol process, which utilizes the CO_2 in the biogas stream fully.

Nevertheless, such compromise design solutions, represented by utilizing a biogas-based system with full CO_2 use, can only be considered for tackling GHG emission mitigation, if the methane leakages are minimized. The importance of reducing methane emissions is already recognized in the EU Methane Strategy from the European Commission (EC, 2020e), which defined actions aimed improving the measurement, reporting, independent control and legislation related to methane emissions. Recently, the European council and parliament have agreed on a regulation to cut methane emissions in the oil, gas and coal sectors in line with the initiatives of The Oil & Gas Methane Partnership (United Nations Environment Programme (UNEP) and Oil And Gas Methane Partnership 2.0 (GMP), n.d.) and The Global Methane Pledge (Global Methane Pledge, n.d.), however, the biogas sector is not included (Council of the EU, n.d.). If these actions would not extend to the biogas production, or prove to be ineffective and the transition to renewable production continues to be desired, either the full costs of the power-to-methanol system need to be accepted or alternative utilization routes for biomass streams where no methane is produced need to be considered (e.g. gasification).

The results for the 2030 cost scenario show that the two pathways of methanol production (or the sector coupled production systems) are projected to be comparable in terms of costs. Eventually, the costs for the power-to-methanol process, may even drop below the biogas pathway, making it the most land- and cost-efficient. However, the recent economic developments leading to increased interest rates, disadvantage the capital intensive power-to-methanol pathway (see sensitivity analysis to interest rate in Supplementary Material B) relative to the biogas pathway, making the projected cost-reductions more uncertain. Therefore, including a second objective function into the design can continue to be influential and political regulations pushing towards efficient land use could have a significant effect on the design of future production systems.

The modeling results also inform about important technologies, which can lead to land-use reductions and synergies in the sector-coupled designs. Introducing wind turbines as part of these production systems has shown to be especially beneficial, as they have a small land requirement and can produce electricity relatively cheaply under the studied renewable energy conditions. Nonetheless, the effect of complementarity of solar energy as an additional source has been observed in the sector-coupled designs with 2030 costs, even if the studied location could be classified as wind-dominant – an effect also observed in Ramirez Camargo et al. (2022). This is pointing out the importance of including solar technologies in the design scope even for wind-dominant locations.

The results also suggest that utilization of wheat straw can already be competitive, improving the economics and reducing the direct land use of such production systems (which is also projected for the 2030 cost scenario). Deploying it as part of industrial production is further supported by the fact that a large-scale wheat straw-based biomethane plant is already operating in Germany (DG Clima, n.d.). The effect of wheat straw utilization is however limited if the size of the wheat production in terms of cost is kept comparable to the costs of the methanol plant, as assumed in this work (more can be utilized only from a relatively larger wheat production system). Nonetheless, the promising results from initial field tests of wheat straw utilization with digestate return warrant further study into its long-term effects on soil quality.

On the other hand, the agrivoltaic technology, which can further intensify the use of agricultural land, was shown to be too expensive under the studied renewable energy conditions – even with a similar drop in costs assumed as expected for the PV modules until 2030. It was only selected to be installed in the most land-intensive (yet extremely costly) designs. An incentive structure to support this technology would thus be needed, yet setting it up in such a way that biomass and electricity are co-produced, and not either one of the them alone for purely economic benefit, is not trivial (Scharf et al., 2021), and calls for further multi-disciplinary research on the boundary between engineering and political sciences.

5.2. *Political optimization*

The analysis in this study revealed where and how political framework conditions can be critical for the choice of a certain process network design for the defined context and example location. The optimal design from a technological point of view, identified in model calculations and based on objective numbers, however, is not necessarily the best choice when it comes to the actual implementation of a production plant in the real world. *Political conflicts* between stakeholders, a lack of *societal acceptance* for elements in the design or the production plant as a whole and the availability and choice of *political instruments* are decisive factors for the successful implementation and operation of such a facility. Aspects regarding the role of political optimization are thus discussed in the following with regard to central results of the modeling study.

The considerations about political framework conditions in Germany and the European Union in the policy analysis have shown that post-fossil industrial production processes are strongly supported and to some extent even explicitly and bindingly demanded. Various subsidy programs have already been introduced or are currently being developed to support the mainstreaming of renewable energy and renewable carbon. Competing claims for land use will continue to exist and against the background of plans to expand nature conservation areas, of progressing climate change and the resulting loss of available land resources, the utilization pressure for land will most likely continue to rise in the future.

In our study, we focused on cost-efficient and land use-efficient designs. Land use conflicts between protecting climate and nature are quite present in the political sphere and have been studied from different scientific perspectives in the past (Steinhäußer et al., 2015; Koven et al., 2022; Purkus, 2016). Conflicts of goals between economy and ecology, but also between global climate protection and local nature conservation (Blöbaum et al., 2023) play a role in this context and are being debated among others in the bioeconomy debate (Böcher et al., 2020; Otto et al., 2021; Beer, 2022). In the past two decades, both in the European Union and in Germany, there have been conflicts and debates on the environmental impacts of policy support for bioenergy and the cultivation of energy crops (*ILUC* Debate, *Food* vs. *Fuel* Debate, *Maizification* Debate) (Böcher et al., 2020; Vogelpohl et al., 2022; Beer, 2022; Purkus, 2016; Otto et al., 2020).

There is a strong tendency today to shift from the use of agricultural crops and biogenic resources from primary production to the use of biogenic residual and waste materials to resolve land use conflicts. Regarding transport costs and the environmental impacts of distributing goods in systems with centralized structures, a shift to more decentralized local and regional production and consumption systems is discussed (Möller et al., 2010; Burger and Weinmann, 2013; Fytili, n.d.). Energy generation in agriculture will probably continue to play a role, but with new approaches that serve multiple goals, as opposed to the strong support and rise of bioenergy made from agricultural crops in the 2000s and 2010s (Beer, 2022; Purkus, 2016). Furthermore, the reduction of direct and indirect GHG emissions from agriculture and the introduction of corresponding pricing and rewarding schemes will play a stronger role in the near future, as recent studies and debates in the EU indicate (European Commission, n.d.). It could be shown in the modeling study, that using wheat straw in a renewable methanol production plant can help to save costs and land. However, there is a conflict of goals between maximizing residual biomass use and conserving soil fertility – and hence between climate protection and nature conservation (Baasch, 2021; Blöbaum et al., 2023; Hagerman et al., 2010; Roberts et al., 2020). Against the backdrop of the high share of agricultural land used for animal feed production, there are debates on the ratio of land used for food, feed and energy plant production and associated possible lifestyle changes. In Germany, 53.6 % of grains produced in agriculture have been used for feed production, 22.8 % for food production and 9.5 % for the cultivation of energy plants in 2021/22 (BLE, n.d.).

From a technological point of view, designs with coupled processes can be cheaper and more efficient regarding land use. But on the other hand, there can be political costs, in the sense that it might be more difficult to find a compromise in project planning and in political processes (Beer, 2022; Roberts, 2000). Conflicts between stakeholders can hinder the implementation of an optimal design and a lack of acceptance for certain technologies among the population or political parties can lead to situations in which second-best options and suboptimal designs are implemented (Baasch, 2021; Sonnberger and Ruddat, 2017; Blöbaum et al., 2023). More complexity and a higher number of included actors lead to more different points of views and interests, and hence more need for coordination and negotiation between stakeholders. This requires new ways of steering and governing, which is discussed in debates on *wicked problems* and *social messes (*Beer*, 2022;* Roberts et al.*, 2020;* Roberts*, 2000;* Ritchey*, 2011;* Balint et al.*, 2011)*. In such complex situations, compromises need to be found and political decisions need to be made on which goals to prioritize and which routes to take. The political regulation of coupled systems can furthermore be complex due to scattered existing regulations and responsibilities. In a system design that integrates several sectors like food, heat, power and methanol production, multiple political resorts are in charge and need to coordinate their activities. Hence, policy integration is crucial for the transition towards more sustainable production systems in the chemical industry. For these reasons, it can be better for the implementation of a project to choose a system design that is not optimal from a technological point of view, if this system design has a higher chance to be accepted and quickly implemented regarding the political framework.

Furthermore, there can be barriers that result from a lack of societal acceptance. This has been observed for the example of wind energy and other fields (Sonnberger and Ruddat, 2017; Fytili, n.d.; Merten et al., 2022). In many cases, wind energy projects have been rejected by local residents and groups (Reitz et al., 2022). A lack of acceptance can also be a barrier for certain technologies in the political arena. In Germany, the Bavarian government introduced the so-called 10H-Regulation (see Supplementary material A). This regulation defined rules about obligatory distances between wind turbines and settlement areas and led to a de facto standstill of wind energy expansion in this federal state. For the case of wind, the model calculations clearly showed the disadvantages of not including wind turbines in the system. Wind energy is comparably cheap and land-efficient, but technology options (and political instruments) are not politically neutral and can be preferred or rejected based on party politics, values, and ideologies (Böcher, 2012; Böcher and Töller, 2015).

We argue based on these experiences that doubts and rejection of new technologies and strategies must be expected also for the introduction of carbon capture technologies or agrivoltaics. Unforeseen dynamics in political and societal processes can lead to scenarios in which some technologically and economically optimized system designs might not be an available option in practice. We showed that with the use of coupled production systems and the combination of established and new technologies, it is possible to save not negligible amounts of land with minor additional costs. The question how many additional costs exactly are acceptable to save a certain amount of land, however, needs to be negotiated for each context by the involved stakeholders and decision makers. If a transition to a post-fossil society is aspired and land resources are limited, additional costs have to be accepted to a certain degree, if local production systems are preferred. However, it is possible to influence the financial aspects with economic policy instruments. Policymakers need to find a balance between the choice of strong policy instruments, that might have an unintended psychological effect, and soft instruments, that lead to weaker regulations, but might still be more effective, if they result in more acceptance.

There are several options for policy instruments that can change the framework conditions for our scenario. It has been stated above that regarding the costs, the renewable methanol production systems calculated are not competitive yet compared to fossil-based systems. This could change with a stricter carbon pricing scheme. From the perspective of climate mitigation and emission reductions, a higher pricing of GHG emissions is desirable. However, these higher prices can lead to new conflicts of goals between climate mitigation, social justice, and the international competitiveness of the industry, as it could be observed in recent political debates for the example of Germany (UBA, 2023; UBA, n.d.). The course for the GHG emission pricing scheme for upcoming years in Germany will be set among others with the introduction of the EU ETS II in 2027, which will first and foremost replace German national regulations in the building and transport sector (Agora Energiewende and Agora Verkehrstwende, 2023).

New options for more land-efficient systems have been identified, like the use of agrivoltaics and the DAC technology. As these options are land-efficient, but costly, financial support programs or obligations can be introduced to give incentives for the operators to use these technologies and save land areas. The use of wheat straw as bio-based residual material is an option that is available today, but it is not yet common in Germany, whereas other countries, first and foremost Denmark, have implemented strategies to push the use of straw as energy source already years ago (Bentsen et al., 2018; Nguyen et al., 2013; Venturini et al., 2019). As the study has shown, the use of wheat straw meets the targets defined in bioeconomy strategies (use of residual biomass) and has been proven to lead to advantages regarding the costs and the land use in our renewable methanol production system. Also for the heat pump technology, advantages for the optimized system design have been shown.

Political regulations will be relevant when it comes to the implementation of renewable production systems in the upcoming years (Böcher, 2012; Barnea et al., 2022). New technology options and their regulation need to be integrated into an existing regulatory framework. It has been shown that agrivoltaics can contribute to more land-efficient production systems and that subsidies for agrivoltaics can be desirable, but their introduction in an existing agricultural system will in any case lead to a change in previous agricultural production orders. As shown for the example of emissions trading, the basic assumptions used in the model and concrete variables can change with the introduction of new political instruments (Barnea et al., 2022; Rozenberg et al., 2014). Carbon capture technologies are rather new and do not yet have a history comparable to renewable energy technologies in public and political debates. Many citizens are not familiar with the concept and available technologies (Blöbaum et al., 2023). It can be assumed that there will be a rejection of new technologies to a certain degree, while at the same time there will be actors that look for solutions for societal problems in new technologies (Sonnberger and Ruddat, 2017; Purkus, 2016; Reitz et al., 2022). Although still costly, the Pareto front comparisons in Fig. 14 show that without DAC the 40kt/year methanol-only production system cannot be built without a land requirement lower than roughly 30 km^2 as the CO_2 has to be sourced from land intensive biomass production. Sector coupling could serve as a strategy to alleviate this dependence as the CO_2 streams resulting from producing other products could be utilized, but at the price of the already mentioned complexity bound with increased number of stakeholders.

It has been shown in political science studies for several fields of environmental policy that coincidences and process inherent dynamics in political processes can play a crucial role and influence policy outcomes (Vogelpohl et al., 2022; Beer, 2022; Böcher, 2012; Böcher and Töller, 2015). We discussed conflicts, debates and negotiation processes that can be expected. We argue that including societal and political factors into the model calculations and the interpretation of the results is necessary, as these factors are decisive for a successful practical implementation and hence for the overall transition process of the chemical industry. A next step that builds on the results generated in this study hence could be the quantification and integration of the societal context into the equations in the model with additional variables.

5.3. Societal goals

Overarching societal goals (Fig. 16) in the fields of climate and biodiversity protection are guard rails for the sustainability transition of the European economy and form the frame for this interdisciplinary study. Associated developments are decarbonization and electrification of processes on the one hand (shift to non-carbon-based processes and products), and defossilization and biologization on the other hand (renewable carbon-based processes and products).

The policy analysis showed that political goals of international climate and biodiversity policy have been translated into more ambitious and more binding political regulations in recent years. After the definition of climate goals on international level in the Paris Agreement in 2015, both the European Union and the German government – as well as other governments – have passed climate laws with binding regulations for climate change mitigation in recent years. Court cases in which governments or other organizations are sued for inadequate climate protection are no longer a rarity. In the multi-level governance system in Europe, policies on international and European level are exerting more and more pressure on national governments. The increased pressure from the superordinate level also applies to national governments and sub-national governments, as the example of Bavarian regulations for wind turbines shows. With the Russian invasion in Ukraine in February 2022, geopolitical arguments for phasing out the use of fossil fuels became more obvious and present in the public debate.

How political instruments in this context can influence economic equations has been shown with our model for the example of carbon pricing mechanisms in the post-analysis. Our calculations confirmed that the impact of carbon pricing on the equation is relatively small with the current prices. A challenge that is currently debated intensely in this context is the conflict of goals between emission reduction with carbon pricing and the aim of social justice. Germany for instance has postponed a planned increase of the carbon price from 2023 to 2024 to unburden citizens and companies during the energy crisis. Conflicts of goals like the latter and trade-offs that we revealed with our study illustrate that social negotiation processes need to take place and political decisions need to be made to successfully manage the shift towards a sustainable economy.

With the publication of the Global Biodiversity Framework in 2022, there has been an agreement on biodiversity goals on international level, which is comparable to the climate goals in the Paris Agreement. It can be expected that the goals of the biodiversity framework will be translated into more binding laws on different political levels in the near future, like it happened in climate policy after the Paris agreement. The recent agreement on biodiversity goals further strengthens our basic assumption that land-efficient systems will be needed in the future due to increasing land use conflicts. Regarding political goals for land use analyzed in this study – e.g. international goals for biodiversity protection and national goals for on-shore wind energy in Germany – associated regulations apply to large areas of land as a whole, like marine areas worldwide in the 30 × 30 targets or Germany as a whole for the 2 % on-shore wind energy goal. Concrete limitations to land availability have not been fed in the model calculations in this study, as percentage targets for the reduction of land use are defined for large regions and not for concrete production sites. However, our results show the implications of different percentages of land use reductions for different designs of the process network.

6. Conclusions

Designing a renewable production system of methanol incorporating the biogas- and the power-to-methanol paths while considering the dynamic behavior of the renewable resources has shown how these pathways can complement each other for cost- and land-efficient production system development. However, the production costs for such renewable systems are still higher than for the ones using fossil feedstock and are hence not yet competitive if only economic objectives are considered. Taking into account politically defined goals, multiple objectives and possibilities to influence the system with regulatory and economic instruments increases complexity and opens up various options for action that imply different trade-offs. From the results of our study on technological optimization, conclusions for the development and implementation phase of renewable production systems can be derived, of which we want to highlight the following five:

First, it was shown that sector coupling of the proposed renewable methanol production with residential electricity, residential heat and food production leads to non-negligible savings of both production costs and land use compared to stand-alone production systems of these products, yet it is inherently bound to technical as well as political complexity. Second, methanol has shown to be useful not only as a product, but also as an energy carrier where its use as a buffer for the seasonal fluctuations of energy demand (mainly wheat grain drying during the harvesting period). Third, including land-use minimization as the second objective function has shown that land-use can be reduced with relatively little cost increases for the biogas- and power-to-methanol pathways under the 2018 and 2030 cost scenarios, with the biogas-based design utilizing the CO_2-waste stream fully with electricity supplied from wind and solar energy representing a potential compromise solution. Fourth, using the biogas pathway to fulfill the goals of reducing GHG emissions can only be done under strict control of methane leakage rates. Fifth, even if wind turbines were the dominant technology leading to land-use reductions under the studied renewable resource conditions, utilization of wheat straw was shown to be beneficial for both reducing the production costs as well as the land requirements. On the other hand, agrivoltaic solar energy generation was only selected in the most land-intensive designs with strict limits on land use, which is difficult to realize with political instruments in the real world. An incentive structure supporting agrivoltaics is thus needed if the efficient utilization of agricultural land that it can achieve is aspired.

The integrated chemical engineering and political science perspective of this study allowed the derivation of additional conclusions concerning the political and societal context, of which we want to highlight the following three: First, designing renewable production systems takes place within a contested political surrounding. Political frameworks function as enabling or restricting institutional factors and new policy instruments, which need to be integrated into an existing regulatory framework, can have a decisive influence on the results of the calculations (e.g. via incentives, taxes). Second, optimization models can inform policymakers, as they allow the assessment and comparison of different design options and illustrate their implications regarding costs, land use, or GHG emissions. Third, optimization models can be developed further and cover more dimensions, become more practice-oriented and more adjusted to specific regions with the incorporation of additional political and societal factors, which we recommend for further studies in the field of renewable methanol production specifically and for further studies in the field of sustainability transitions of the chemical industry in general.

CRediT authorship contribution statement

Tibor Svitnič: Conceptualization, Methodology (Modeling study), Investigation (Modeling study), Software, Writing – original draft (Introduction, Modeling study, Discussion: Technological optimization, Supplementary material B and C), Writing – review & editing, Visualization.

Katrin Beer: Conceptualization, Methodology (Policy analysis), Investigation (Policy analysis), Writing – original draft (Policy analysis, Discussion: Political optimization, Societal goals, Supplementary material A), Writing – review & editing.

Kai Sundmacher: Conceptualization, Supervision, Writing – review & editing.

Michael Böcher: Conceptualization, Supervision, Writing – review & editing.

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Declaration of competing interest

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

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