Abstract: While some studies have simultaneously modeled the competitiveness of biochemicals alongside bioenergy and biofuels for greenhouse gas abatement, this has never been done before for Germany. The findings on the potential greenhouse gas abatement from these previous studies cannot be replicated in the German context because of different frame conditions, such as biomass potentials, temporal horizon, climate targets and the evolution of demand from biomass end-use sectors. This, therefore, necessitates a country-specific assessment. In this study we use a bi-objective bottom-up optimization model to quantify the potential greenhouse abatement (i.e. from best compromise solutions between the cost-optimal and technical-optimal objectives) for biomass deployment to the bioenergy, biofuels and biochemical sectors of the German bioeconomy. Results show that, with a reference crude oil price development, biomass potentials (i.e. 300 petajoules of forest residues and 2.7 million hectares of arable land) could save 69 million t CO_2-eq by 2050, representing a 6% reduction over 1990 GHG emission levels in the energy, building, transport and industrial sectors. The cumulative abatement (i.e. for 2020 - 2050) of 1.72 billion tonnes of greenhouse gas emissions was found to be 8.5% higher than when the available biomass resources were exclusively used for bioenergy and biofuels.

Keywords: Bioeconomy, bioenergy, biochemicals, multi-objective optimization, biomass allocation scenario analysis

1. Introduction

There have been growing calls for concerted action against global warming and climate change (Wahlström et al. 2019; UN 2019). Against this backdrop, the international community adopted the Kyoto protocol in 1997 (UN 1998) and more recently the Paris Agreement (UN 2015) with the aim of limiting the amount of greenhouse gases (GHG) in the atmosphere. As the largest emitter of greenhouse gases in all of Europe–Europe being the third largest emitter in the world (Armstrong 2019)–Germany formulated the Climate Action Plan to embody its commitment as a signatory of the Paris Agreement. The Climate Action Plan sets out climate targets until 2050 (BMUB 2016) and comprises a broad range of mitigation measures in the agriculture, transport, building, industrial, and energy sectors. For the energy, transport and building sectors, the "Energiewende"(energy transition) was specifically devised to represent the country's planned transition to a nuclear-free and low-carbon economy that would cover around 85 - 90% of greenhouse gas reduction by 2050 relative to 1990 (Agora Energiewende 2017; Federal Republic of Germany Foreign Office 2015).

Energy scenarios, which explore different transformational pathways towards reaching German climate targets, indicate that biomass will play a relevant role in the future (Szarka et al. 2017; Samadi et al. 2018). Biomass is a multifaceted renewable resource that can undergo biological, chemical and thermochemical conversion steps to produce power, heat, biofuels and biochemicals (Tursi 2019). Even though biomass is a renewable resource, its annual potential is limited due to land use constraints (Jering et al. 2013), technical constraints, ecological restrictions and forest management sustainability principles (Aust et al. 2014). Therefore, as a result of the annual limited availability of biomass and the versatility of its applications, an understanding of its optimal allocation is required in order to capture maximum benefit.

Studies have assessed the contribution of biomass resources towards replacing fossil counterparts (see Table 1). The assessment models applied in these studies differ in terms of their:

- approach, i.e. top down (Masui et al. 2006) or bottom up (Millinger 2019; Jordan et al. 2019),
- spatial scope, i.e. global (Azar et al. 2003; Gielen et al. 2003; Daioglou et al. 2015), national (Millinger et al. 2017; Tsiropoulos et al. 2017) and municipal (Saghaei et al. 2020; Malladi and Sowlati 2020) and
- temporal horizon, i.e. long term (Daioglou et al. 2015) medium term (Millinger and Thrän 2018) and short term (Tsiropoulos et al. 2017; König 2011)).

Table 1: Current studies on biomass deployment for GHG mitigation

Spatial scope		Source	Bioenergy or biofuels	Bioenergy, biofuels and biochemicals	Single objective	Bi-objective
Municipal		Malladi and Sowlati (2020)	✓	x	x	✓[1,2]
		Saghaei et al. (2020)	✓	x	✓	x
National	Germany	König (2011)	✓	x	✓[1]	x
		Jordan et al. (2019)	✓	x	✓[1]	x
		Millinger and Thrän (2018)	✓	x	✓[1]	x
		Millinger (2019)	✓	x	✓[2]	x
	Other	Tsiropoulos et al. (2017)	x	✓	✓[1]	x
		Berntsen and Trutnevyte (2017)	✓	x	✓[1]	x
		Panos and Kannan (2016)	✓	x	✓[1]	x
		Hugues et al. (2016)	✓	x	✓[1]	x
		Chiodi et al. (2013)	✓	x	✓[1]	x
Global		Daioglou et al. (2015)	x	✓	✓[1]	x
		Azar et al. (2003)	✓	x	✓[1]	x
		Zhao et al. (2015)	✓	x	✓[1]	x

The ✓ indicates a "yes" and the superscripts [1 and 2] represent the minimizing objectives of cost and GHG emissions respectively. The x indicates a "no".

Although efforts have previously been made to simultaneously assess competition between bioenergy, biofuels and biochemicals for biomass (Daioglou et al. 2015; Tsiropoulos et al. 2017), this has not been done specifically for Germany. In (Daioglou et al. 2015), competing uses of biomass for energy and chemicals were assessed for the whole world up to the year 2100. Tsiropoulos et al. (2017), on the other hand, took a national approach and assessed the role of biomass in bioenergy and biochemicals for the Netherlands from 2010 to 2030. However, due to the different frame conditions, such as biomass potentials, temporal horizon, climate targets and the evolution of demand from biomass end-use sectors, these studies are unable to provide a clear picture of the potential for GHG abatement from biomass in the German context.

Table 1 shows that current knowledge regarding the contribution of biomass potentials towards GHG mitigation in Germany has been limited to the bioenergy and biofuels sectors. Furthermore, the current studies only consider single objective functions (i.e. minimizing costs and GHG emissions) in their models. For example, König (2011) used the optimization model TIMES to show cost effective biomass technologies in the heat, power and transport sectors that could contribute to German climate targets. This was done using cost minimization as the objective function and 2005 - 2030 as the temporal scope. The approach used by Jordan et al. (2019) is similar to that of König (2011), however it only considers the heat sector. Millinger et al. (2017) and Millinger and Thrän (2018) used a cost minimization approach to present competitive biomass technologies in the transport sector, while the approach of Millinger et al. (2019) shifted to maximizing GHG abatement.

While these studies have helped shape knowledge concerning competitive biomass technologies and the contributions towards German climate targets, the results could be sub-optimal especially considering that biomass has other competing uses, such as for biochemicals. Furthermore, the single objective functions included in these studies disregard cost-benefit analyses and the accompanying tradeoffs. Therefore, the goal of our study was to quantify for Germany the GHG abatement potential for biomass by considering a systems approach where biochemicals are simultaneously modeled with biofuels and bioenergy. The GHG potential is assessed from the standpoint of maximizing GHG abatement (i.e. technical potential) and cost optimization in order to determine the tradeoffs that may arise. According to the authors, this has never been done before. The following questions were considered:

- What are the potentials and implications on the status quo in Germany if there is additional GHG abatement from biomass resources beyond the energy system?

- Does an allocation of biomass based on cost optimization conflict with the technical GHG abatement potential?
    - If yes, what is the tradeoff and what could be the best compromise solutions?

2. Materials and methods

In order to investigate the possible contribution of biomass potentials towards German climate targets, a mathematical optimization model was developed that builds on the BENOPT optimization model (Millinger 2019). The model is mathematically programed using the General Algebraic Modelling System (GAMS) and interacts with Matlab, where data is prepared and results are visualized. Figure 1 shows the process diagram for the methodological steps involved in the study. Exogenous data—i.e. detailed techno-economic data for the technologies under consideration, life cycle inventories and the cost of feedstock cultivation, biomass potentials, conversion capacities, sectoral demands etc. (Table 5 and Appendices A - C) are imported from an excel spreadsheet using Matlab. Life cycle GHG emissions and costs are calculated in Matlab using the imported data. Additionally, parameter values are interpolated and converted into a format that can be handled by GAMS. After the data has been prepared, it is transferred to GAMS using a GAMS Data Exchange (GDX) file. In GAMS, the main model is created and the optimal allocation of biomass is calculated based on maximizing GHG abatement (i.e. the technical potential for GHG abatement) and minimizing system costs, under, capacity, biomass potentials and sectoral demand constraints. The optimization results are imported in a text file into Matlab, where the data is visualized.

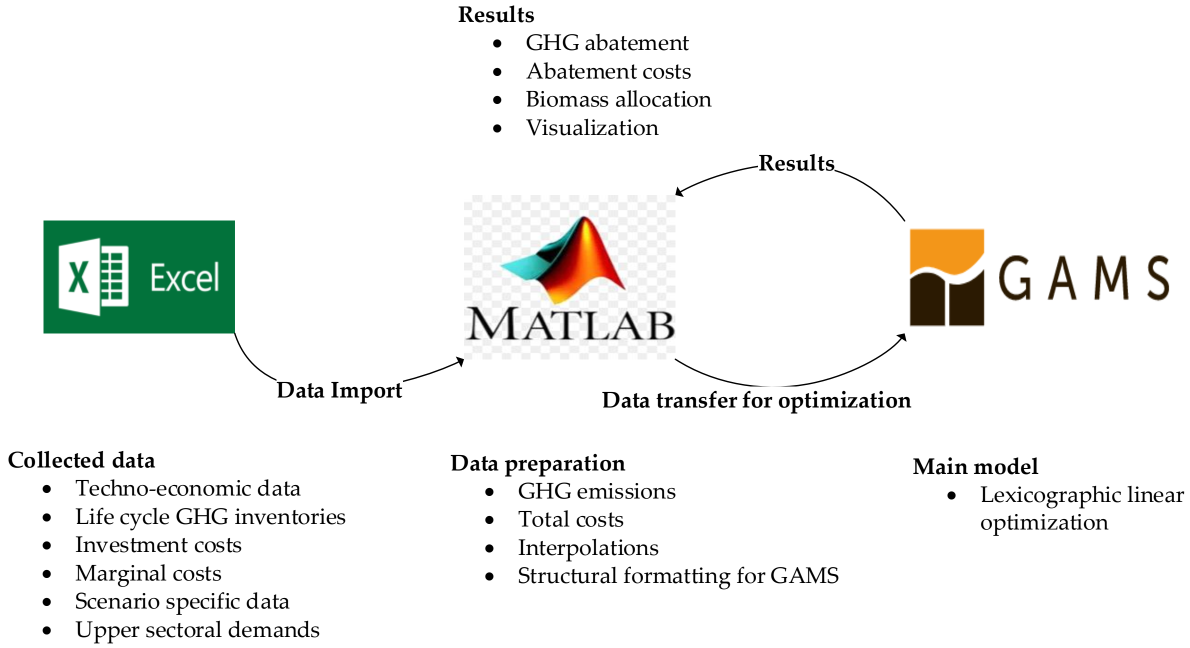

Figure 1: Process diagram of the methodological steps

2.1. Description of the main model

The developed model is a deterministic bottom-up linear optimization model with perfect foresight that encompasses biomass crop cultivation, conversion processes and sectoral demands. In the model, bioenergy, biofuels and biochemical technologies compete for biomass potentials from 2020 to 2050 based on maximizing greenhouse abatement and minimizing system costs. The competition for biomass is constrained by current conversion capacities, available biomass resources and sectoral demands. The resulting model in GAMS has 9,571 equations and 11,362 variables. This represents an underconstrained model with 1,791 degrees of freedom. Figure 2 is an illustration of the model's conceptual framework showing the biomass potentials, technologies and sectors.

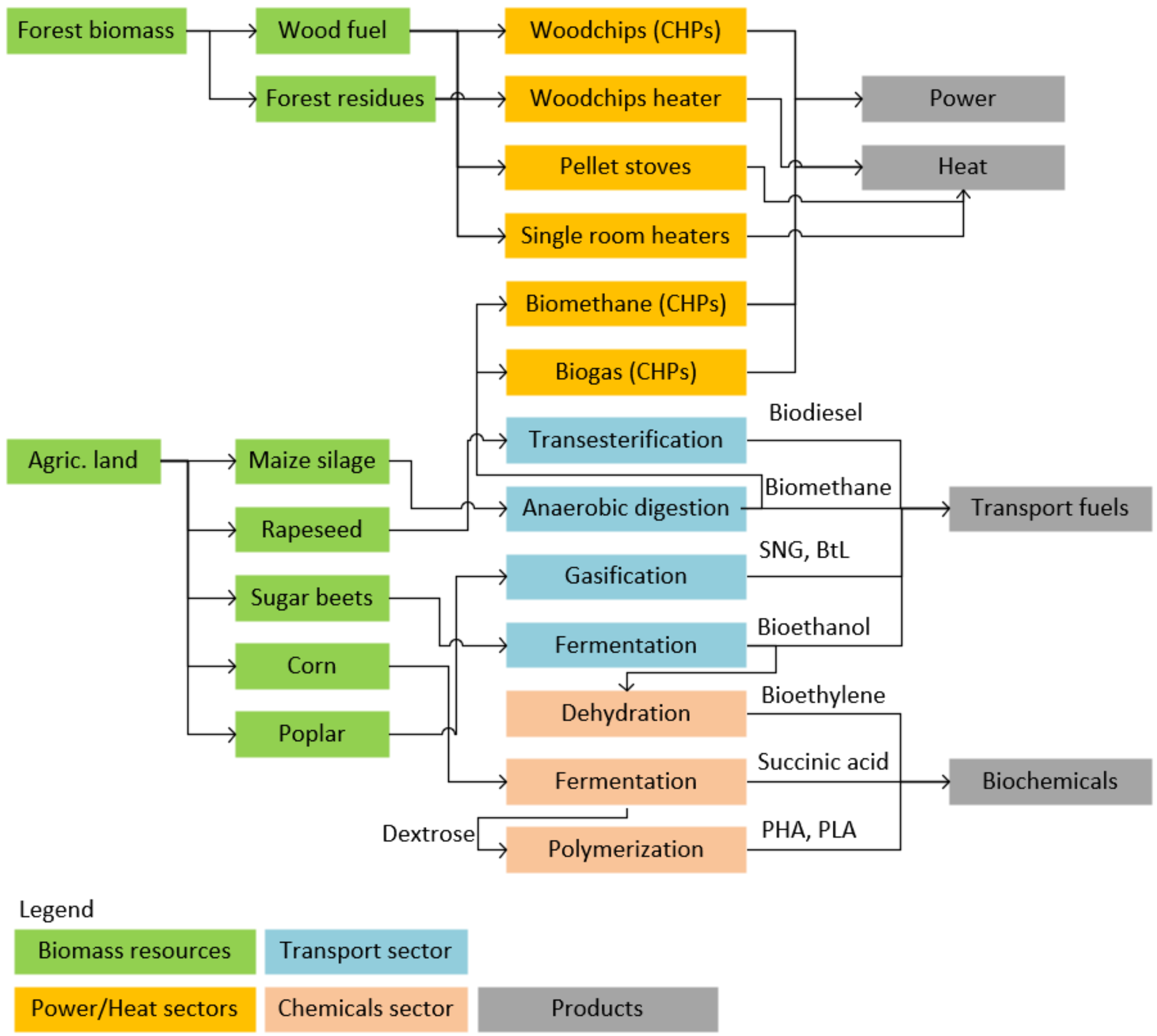

Figure 2: Simplified modeling framework. Here CHPs stands for combined heat and power plants, SNG stands for synthetic natural gas, PHA for polyhydroxyalkanoates and PLA for polylactic acid.

2.1.1. Objective functions

Biomass allocation was investigated based on maximizing GHG abatement in order to determine the technically feasible GHG abatement from biomass potentials. At the same time, cost minimization was also investigated because, in a market-based economy like Germany, allocation of resources is premised on the maximization of welfare by the economic actors. As economic actors, the producers of goods and services achieve this by minimizing costs.

The objective function for the cost optimal biomass deployment (εp) is the difference between the market price for the fossil references ($\mathrm{P}_{sub,t}$) and the total cost of production ($\mathrm{TC}_{i,t}$) for the bio-products, multiplied by production ($\pi_{i,t}$), which is in petajoules (PJ) for bioenergy options and tonnes (t) for biochemicals. This is added up over the entire timespan and for all technology options (Equation 1). The subscript *i* represents the technological options, while *t* represents the yearly modeling time points (i.e. 2020 to 2050). The market price developments of the fossil reference are described in detail in Section 2.3.3. Total costs include the marginal costs (i.e. the feedstock costs and operation and maintenance costs minus co-product income) and investment costs. Technology-specific cost data and other data are shown in Appendices B and C.

$$\varepsilon p = \sum_{i,t} (\mathrm{P}_{sub,t} - \mathrm{TC}_{i,t}) * \pi_{i,t} \qquad (1)$$

The GHG abatement objective function (ε) is the difference between the life cycle GHG emissions for the fossil reference technology ($\varepsilon_{sub,t}$) and the life cycle GHG emissions for the bio-product $\varepsilon_{i,t}$, multiplied by the bio-product production and added up over all technological options and for the entire timespan (Equation 2). The GHG emissions for the bio-products equal the sum of GHG emissions from feedstock cultivation, transportation, and emissions from using the non-renewable energy in the conversion steps. Detailed data for the GHG footprint calculations is provided in Appendix A.

$$\varepsilon = \sum_{i,t}(\varepsilon_{sub,t} - \varepsilon_{i,t}) * \pi_{i,t} \qquad (2)$$

2.1.2. Constraints

Equations (3) and (4) ensure that the amount of bio-products produced is constrained by the amount of available biomass and available plant capacities. The capacities in the subsequent year ($k_{i,t+1}$) should be less than or equal to the capacities in the previous year ($k_{i,t}$) plus the installed capacities ($k^{+}_{i,t+1}$) minus the capacities that decommission ($k^{+}_{i,t-\ell_i}$) as they reach their end of life (ℓ_i) as shown in Equation (5). Equation (6) ensures that additional annual capacities are limited by a capacity ramp factor. The minimum capacity ramp (r_{min}) is set to 1 PJ for bioenergy and biofuels and 100 kt for biochemicals, while the capacity ramp factor (r_f), which limits capacity expansion to a percentage of the previous year's capacity, is set to 45%. In order to prevent the phasing out of available capacity before it reaches its end of life, the model considers a minimum production of 30%. The sum of the sectoral production should be less than or equal to the total sectoral substitution potential (δ_t), as shown in Equation (7). In Equation (8), the total acreage use per technology is limited by ($h_{i,t}$), whose upper bound is set to 1.37 million hectares. This equals the average maximum acreage use for a single technology for the years 2015 - 2017 (FNR 2019). Equations (9) and (10) ensure that the available biomass is limited by the available agricultural land and forest residue potentials respectively. The decision variables, parameters and scalars for the model are shown is Table 2.

$$\pi_{i,t} \leq m_{i,t} * \eta_i \qquad (3)$$

$$kf_{i,t} * k_{i,t} \geq \pi_{i,t} \qquad (4)$$

$$k_{i,t+1} \leq k_{i,t} + k^{+}_{i,t+1} - k^{+}_{i,t-\ell_i} \qquad (5)$$

$$k^{+}_{i,t+1} \leq r_{min} + r_f . k_{i,t} \qquad (6)$$

$$\delta_t \geq \sum_i \pi_{i,t} \qquad (7)$$

$$h_{i,t} \geq m_{i,t} * (\mathrm{Y}_{i,t})^{-1} \qquad (8)$$

$$\Lambda_t \geq \sum_i m_{i,t} * (\mathrm{Y}_{i,t})^{-1} \qquad (9)$$

$$F_t \geq \sum_i m_{i,t} * \mathrm{C}_{i,t} \qquad (10)$$

Table 2: Decision variables, parameters and scalars for the model

Symbol	Description	Type
$\pi_{i,t}$	Bio-products production	Continuous positive
$m_{i,t}$	Available biomass feedstocks	Continuous positive
$k_{i,t}$	Capacities in the previous year	Continuous positive
$k_{i,t+1}$	Capacities in the subsequent year	Continuous positive
$k^{+}_{i,t+1}$	Newly installed capacities	Continuous positive
$k^{+}_{i,t-\ell_i}$	Capacities decommissioned after their end of life	Continuous positive
η_i	Conversion efficiencies	Parameter
$kf_{i,t}$	Technology capacity factor	Parameter
δ_t	Total upper substitution potential	Parameter

$h_{i,t}$	Upper bound for technology hectare usage, set at 1.5 million ha	Parameter
$Y_{i,t}$	Feedstock agricultural yields	Parameter
Λ_t	Available agricultural land for feedstock cultivation	Parameter
F	Available forestry biomass	Parameter
$C_{i,t}$	Calorific value of woodchips and wood pellets	Parameter
r_{min}	Minimum capacity ramp (set at 1PJ for bioenergy and 100 kt for biochemicals)	Scalar
r_f	Capacity ramp factor, set at 0.45 for all technologies	Scalar

2.2. Solution approach for the bi-objective optimization

Multi-criteria optimization refers to mathematical programming models that have more than one objective function with usually no unique optimal solution. As a consequence of having conflicting objectives and different sets of solutions, multi-criteria optimization requires decision support for the best compromise options. Techniques for solving multi-criteria optimization problems vary. Beckmann et al. (1979) classified these methods into three categories based on the stage at which decision makers express their preference.

The first category includes *a priori* methods, in which, as the name suggests, the decision maker expresses a preference before the optimization process is complete. These methods require the decision maker to assign weights to the objective functions based on the importance of the objective functions (Yu and Solvang 2016). Mavrotas (2009) points out that such methods receive criticism because it is very difficult for the decision maker to make a prediction in advance and accurately quantify preferences. The second category of methods are the interactive methods in which the decision maker exchanges phases of dialogue with phases of calculations, enabling the process to converge at the most preferred solution after a few iterations (Mavrotas 2009). The third category consists of *a posteriori* methods, which are the opposite of *a priori* methods. The *a posteriori* methods generate an evenly distributed Pareto front from which the decision maker can choose the preferred solution.

This paper uses a method from the third category and deploys a specific method for visualizing the Pareto front called the augmented e-constraint method which uses lexicographic optimization (Mavrotas 2009).

2.3. Data and assumptions

2.3.1. Feedstock costs and emissions

Feedstock prices for energy crops (i.e. maize silage, corn grains, sugar beets, rapeseed, poplar and miscanthus) were estimated using the methodology described in (Millinger and Thrän 2018). The per hectare profit from wheat (benchmark crop) was added to the per hectare production costs of the energy crops to produce estimated feedstock prices. An annual price increase of 2% was assumed for wheat. The total feedstock costs were then determined by adding the cost of transportation to the feedstock price. The cost of transportation for Germany of 0.88 $€_{2020}$/km/t was used as well as an assumed average distance of 20 km (Ruiz et al. 2015). However, the calculated transportation costs vary due to the fact that feedstocks have different energy densities and water content.

The selling price for corn stover, which was used as a credit for corn grain cultivation, was calculated from the cost of corn grains using Equation 9. The value 0.175 is the ratio of the mass of corn grains to the mass of the whole plant on a dry weight basis.

$$\alpha = 0.175\beta + \mu \qquad (9)$$

Where
α is the price of corn stover in €/t_{DM}
β is the price of corn grains in €/t_{DM}

μ is the cost for harvesting and storing corn stover which is taken from (Paulson and Khanna 2016).

For woodchips and pellets, the natural gas price projection according to the EIA "reference oil scenario" (EIA 2019) was used as a proxy. This is because, according to C.A.R.M.E.N (2020), the prices for woodchips and pellets follow the price of natural gas in Germany. Because woodchips and pellets have higher energy densities than the energy crops considered here, an average annual distance of 60 km and a transportation cost of € 0.88 €$_{2020}$/km/t was assumed (Ruiz et al. 2015).

The GHG emission factor for woodchips used in the power and heat sectors was adapted from (Virbickas and Kliopova 2017). For wood pellets, the GHG emission factor was calculated based on inventory data from Nunes et al. (2014). Data for GHG inventories from agriculture for different energy crops is shown in Appendix A. GHG emissions resulting from feedstock transportation were also taken into account. Emissions from fertilizers were assumed to fall 15% by 2035 and 25% by 2050 relative to the base year.

2.3.2. Biomass potentials

In 2016 and 2017, 2.7 million hectares of arable land were used to cultivate energy crops in Germany (FNR 2019). This value was used as input data for the model and remained constant until 2050. Furthermore, 75% of the annual technical potential of forest residue, equaling 225 PJ (DBFZ 2015; Brosowski et al. 2016), was used in the model, and this grows linearly to 100% by 2050. In this context, the technical potential includes restrictions such as technical limits on biomass collection and other competing uses and legal regulations (Brosowski et al. 2016).

2.3.3. Market prices

The linear regression equations used to estimate market prices for biochemicals and biofuels are shown in Table 3. The development of the crude oil price (which was used as a proxy for estimating price dynamics for fossil reference chemicals and gasoline) was taken from the "reference oil scenario" (EIA 2019). The price developments for electricity and heat (Table 4) were taken from (Thrän et al. 2019). All the data for projecting market price developments have been adjusted to the 2020 value of the euro in order to facilitate a fair comparison.

Table 3: Market price estimation equations

Bio-product	Fossil reference	Regression equation	Units	Source
Bioethylene	Ethylene	$y = 7.3x + 572$	€/t	(Seddon 2012)
Succinic acid	Adipic acid	$y = 26x + 67$	€/t	(Straathof and Bampouli 2017)
PLA and PHA	Polystyrene	$y = 9.5x + 794$	€/t	(Seddon 2013; Franco and Thorsnes 1999)
Biofuels except biodiesel	Gasoline	$y = 0.13x + 39$	€/GJ	(Sönnichsen 2020b)
Biodiesel	Diesel	$y = 0.15x + 26$	€/GJ	(Sönnichsen 2020a)

PLA stands for polylactic acid, PHA for polyhydroxyalkanoates, y for the market price of the bio-products, and x for the price of crude oil in $/barrel.

Table 4: Development of electricity and heat prices

		2020	2030	2040	2050
Electricity price	ct_$_{2020}$/kWh	19.1	20.9	22.8	24.7
Heat price	ct_$_{2020}$/kWh	7.7	9.4	11.2	13.0

2.3.4. Upper sectoral demands

The "Verband der Chemischen Industrie" (Association of Chemical Industries) projected a 1.8% annual increase in production until 2030 in their base scenario for the development of the chemicals industry (VCI 2012). This annual increase, which caps the production of individual biochemicals, is considered in this paper until 2050. For bioenergy and biofuels, the upper sectoral production limits were taken from the 95% GHG emissions reduction scenario for Germany (Thrän et al. 2019) (Table 4).

The production of PLA for the year 2018 in Germany was 500t/y (European Bioplastics, personal communication, April 29, 2019). Based on a 90% plant availability, a 555t/y capacity was used for PLA for 2020. Bioethylene, succinic acid and PHA currently do not have production capacities in Germany.

Table.5: Biomass demand by sector

Sectors	Unit	2020	2050
Power	TWh	47	19
Industrial heat	TWh	51	71
Household heat	TWh	52	38
Trade and commerce (heat)	TWh	11	0
Transport fuels	TWh	58	141

2.3.5. GHG emissions considerations

The fossil reference emission factors for the power, heat and transport sectors were set at 183, 80 and 90 g CO2-eq/MJ respectively (European Commission 2018). The development of the emission factor of the power mix in Germany was based on the World Wide Fund (WWF) scenario in which coal power plants are decommissioned after a plant life of 20 years and in which there is an ambitious expansion of renewable energies (WWF 2017). In this scenario, all lignite and hard coal power plants have to decommission by 2040. Therefore, in this paper, the fossil reference of 183 g CO2-eq/MJ for the power sector linearly reduces to 80 g CO2-eq/MJ from 2030 to 2040. This scenario was chosen because, unlike the "rapid phase out of coal" scenario, which also includes emissions within the determined emissions budget for the German power sector, it also takes into account the legal feasibility of decommissioning coal power plants.

For the biochemicals sector, bioethylene from sugar beets and lignocellulose biomass replace fossil-based ethylene, and the IPCC default value for the emission factor was used (Neelis et al. 2003). Succinic acid and polylactic acid (PLA)/polyhydroxyalkanoates (PHA) replace adipic acid and polystyrene respectively as in Musonda et al. (2020). The emission factor for adipic acid was taken from (Gatto 2013) and the emission factor for polystyrene from (Ruuska 2013).

The electricity requirements to produce 1 ton of fossil reference chemicals (used to adjust fossil chemicals emission factors as a result of the change in the German power mix) are shown in Table 6.

Table 6: Electricity requirements of fossil references

Biochemical	Unit	Value	Source
Ethylene	kWh/t	842	(Worrell et al. 2007)
Adipic acid	kWh/t	187.8	(Towler and Sinnott 2013)
Polystyrene	kWh/t	207	(Ricart et al. 2011)

The integrated production of biochemicals and the end of life treatment of their end products (recycling and no energy recovery) were found to be key issues for GHG abatement by Musonda et al. (2020). Integrated production involves the use of by-products from biochemicals production to replace fossil resources, thereby accounting for the resulting GHG abatement. This paper assumed integrated biochemical production and the end-of-life recycling (i.e. no energy recovery) of their end products.

2.4. Scenarios

In order to answer the formulated research questions, two scenarios were created and analyzed. In the base scenario, representing the status quo in Germany, biomass is only used for bioenergy and biofuels production. In the biochemicals deployment scenario, biochemicals were also considered alongside bioenergy and biofuels. The upper production limit for biochemicals was assumed to grow linearly, from zero in 2020 to 100% of the production of major base chemicals by 2050. The development of the crude oil price (which was used as a proxy for estimating price dynamics for fossil reference chemicals and gasoline) was taken from the "reference oil scenario" (EIA 2019).

2.5. Sensitivity analysis of crude oil price developments

Based on current laws and regulations that affect the energy sector, the United States Energy Information Agency (U.S. EIA) projected a reference path for how crude oil prices could develop until 2050. Two side cases that represent conditions that could push prices to deviate extremely from the reference path have also been outlined (i.e. low and high oil price projections).

For this paper, in addition to the scenario analyses which are based on the reference crude oil price development, sensitivity analyses were conducted for the "low" and "high" crude oil price developments to determine how the profit dynamic results would change. The price development projections for crude oil are shown in Figure 3.

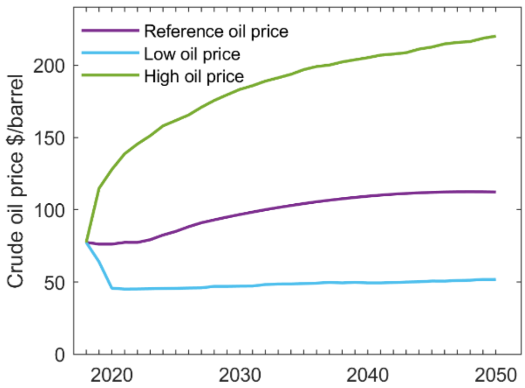

Figure 3: Crude oil price developments adapted from (EIA 2019)

3. Results and discussion

Before the results are presented and discussed, some issues should be pointed out in order to add context to the generated results. We did not consider any regional effects and spatial distribution (i.e. with regard to biomass production or transportation distances along the supply chain). Studies that have previously modeled the biomass supply chain for bioenergy have focused on the municipal rather than national level due to the large computational load of geographical information system (GIS) data (Fattahi et al. 2020). Incorporating this aspect into the model could have provided a better approximation of the overall GHG emissions and costs for the bioproducts.

3.1. Base scenario

Figure 4 shows the GHG abatement for the technologies under consideration for the objective functions of cost and GHG abatement. In the base scenario for both objectives, agricultural land is effectively used for the cultivation of feedstocks for the transport sector. In the cost-optimal objective, bioethanol, biodiesel and biomethane play similar roles for GHG abatement in the base year. Biodiesel plays a short-term role, while biomethane becomes dominant in the medium and long term. In the GHG abatement objective, SNG and biomethane become increasingly dominant in the medium and long term, while bioethanol and biodiesel are only produced in the short term.

For the power and heat sectors, biogas CHP production reduces to zero by 2040, while CHP plants with woodchips play similar roles in both objectives. In the household heating subsector for both objectives, single room heaters are dominant in the short term, while wood pellet heaters become increasingly competitive in the medium to long term. As a result of the assumed complete decomissioning of coal power plants by 2040, which results in natural gas being used as the fossil reference, there is a drop in GHG abatement from 2030 to 2040 for both objectives due to reduced GHG abatement from CHP plants.

These results confirm the previous findings regarding biomass deployment for bioenergy and biofuels in Germany. In the "BIC+GHG" scenario, which depicts competition for biomass from different technologies with production shares not predetermined by legislation, König (2011) showed that biodiesel was not cost competitive in the medium term, while biomethane was competitive. This result aligns with that of Millinger and Thrän (2018) as well as with the results of this study. König (2011) further showed that solid biomass was cost competitive in the heat and power sectors. Jordan et al. (2019) also confirm this finding. These conclusions correspond to our results because, for bioenergy end-uses, annual energy crops have been shown to play a limited role since the production of power and heat for GHG mitigation is effectively done by solid biomass.

3.2. Biochemicals deployment

In the biochemicals deployment scenario and from the perspective of cost optimization, results show that arable land should preferably be used to cultivate feedstocks for the production of succinic acid rather than for biogas and biomethane CHP plants. This is because succinic acid has a higher potential to generate profits per hectare of arable land for feedstock cultivation than all bio-products except biomethane and bioethanol (Figure 5). From the GHG abatement perspective, succinic acid and bioethylene are preferred for biomass utilization over SNG and biomethane from the transport sector. This is because bioethylene and succinic acid are higher in the merit order for biomass allocation in the GHG abatement objective function (Figure 5). The production of biochemicals in both objectives results in 8% more GHG abatement relative to the base scenario.

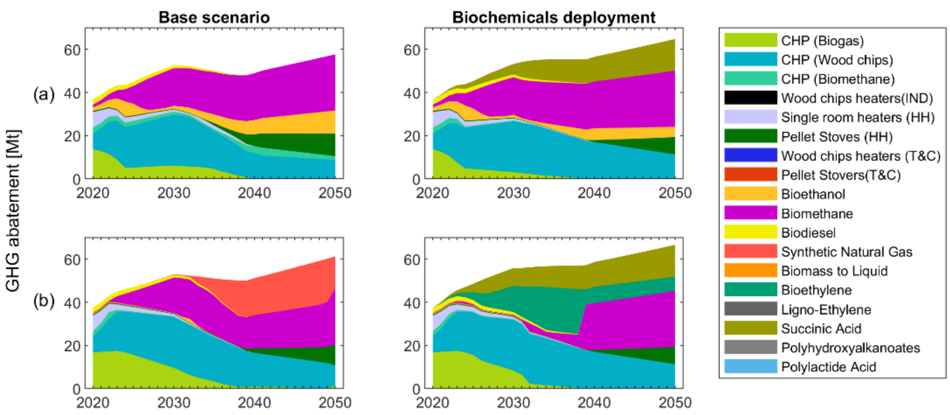

Figure 4: GHG abatement in the cost-optimal (a) and GHG abatement-optimal (b) objective functions for biomass allocation in the base and biochemicals deployment scenarios. Here CHP stands for combined heat and power plant, IND for industry, HH for household, and T&C for trade and commerce.

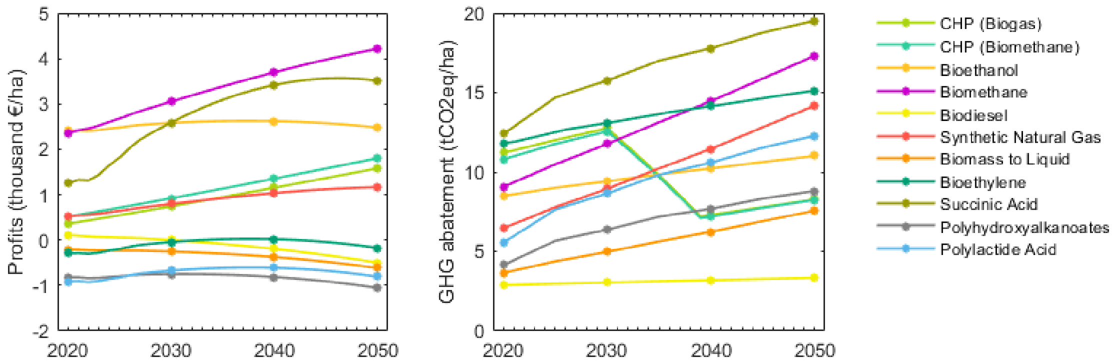

Figure 5: The potentials for profit and GHG abatement developments for biobased technologies with feedstocks from arable agricultural land. Here CHP stands for combined heat and power.

A novel finding from this study is that, while there is potential for additional GHG abatement from the same biomass potentials beyond the German energy system, this is achieved through reduced biomass allocation to the bioenergy and biofuels sectors (see Figure 6). The competition for biomass as a result of the increased deployment of biochemicals is mainly for gaseous biofuels (biogas, biomethane and SNG). Since these biofuels were exclusively produced from maize silage in this study, as a result of the preferred usage of agricultural land for cultivation of feedstocks for biochemicals production, there should be an increase in the use of organic wastes from households, industry and agriculture in order to fill the gap. A further key finding is that solid biomass (i.e. lignocellulose biomass) is not a good option for bioethylene production from. Instead, it is a competitive feedstock for power and heat production, especially when there is an increased production of biochemicals.

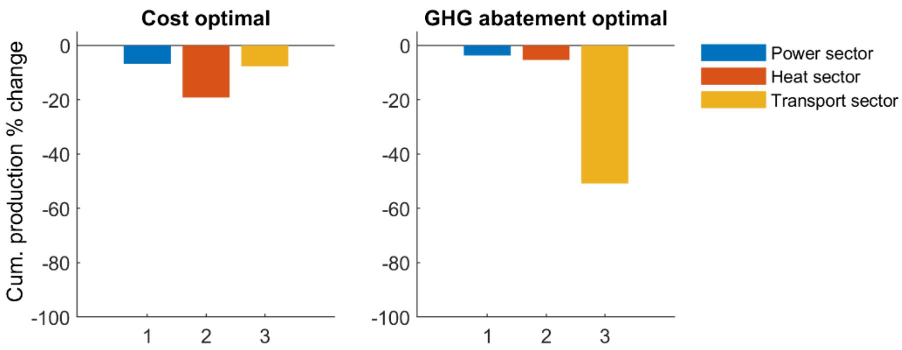

Figure 6: The production percentage changes for the two objectives in the biochemicals deployment scenario.

Furthermore, these results show that the increased deployment of biochemicals in the German bioeconomy, in both the short and medium term, is not limited by biomass availability but by their cost competitiveness in relation to other competing biomass applications. When considering the GHG abatement objective, arable land for cultivating feedstocks is preferably used for biochemicals production and not for biogas CHP plants and SNG in the transport sector. However, from the cost optimal objective, biomass use in the transport sector (i.e. biomethane) remains relatively unchanged. The biochemicals sector and the power and heat sectors compete for biomass potentials as a result of increased biochemicals deployment. Forest biomass, therefore, proves to be most beneficial in the electricity and heat sectors in terms of meeting climate objectives.

Although the underlying assumptions and frame conditions differ between this study and that of Tsiropoulos et al. (2017) and Daioglou et al. (2015) , our results complement their finding that biochemical production could increase in the future.

3.3. Cost optimal biomass allocation conflicts with the technical GHG abatement potential

The results for the Pareto fronts for the two objectives in the scenarios under consideration are shown in Figure 7. As can be seen, Pareto solutions with lower values of total GHG abatement have higher corresponding values of total profits and vice versa. This means that, for additional GHG abatement, investments into relatively more expensive technologies have to be made. Points A1 and A2 represent the cost optimal objective while disregarding the maximization of GHG abatement. On the other hand, points B1 and B2 represent the maximizing GHG abatement objective while disregarding the cost-optimal objective. At points A1 and A2, the total profits generated from biomass deployment are €254 and €280 billion respectively. The corresponding GHG abatement in these cases is 1.54 and 1.66 billion tonnes of CO_2-eq, respectively. In contrast, at points B1 and B2, total GHG abatement increases to 1.59 and 1.72 billion tonnes of CO_2-eq over the optimization period, corresponding to total profits of €213 and €204 billion respectively. The grid points between points A1 and B1 and A2 and B2 represent the different possible compromise solutions between the cost and GHG abatement objectives which a decision maker can choose from depending on the intended goals.

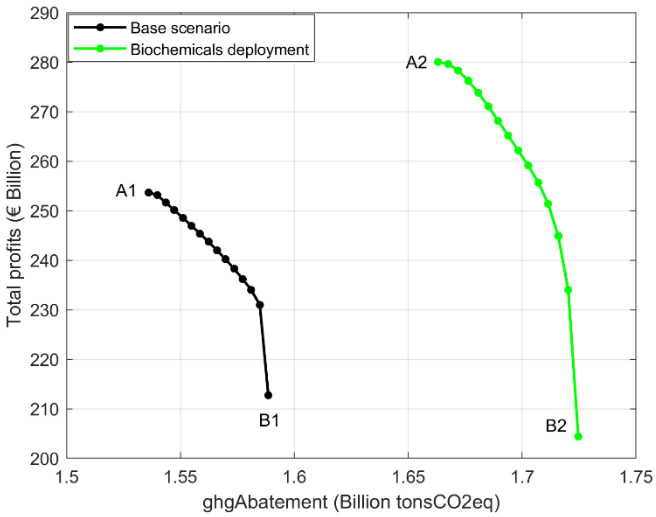

Figure 7: The Pareto optimal curves for the base and biochemicals deployment scenario.

Figure 8 shows additional GHG abatement and the corresponding opportunity costs as one moves from the optimal costs value to the optimal GHG abatement value. For example, at grid point number 14 in both scenarios, the opportunity costs increase sharply with a relatively small increase in the additional GHG abatement. Therefore, grid point number 14 could represent a best compromise solution for the two objective functions.

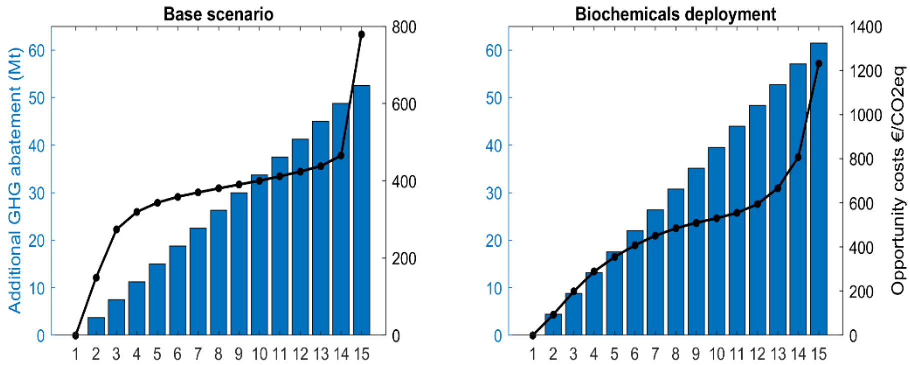

Figure 8: Decision support for best compromise solutions

The interpretation is that, in both scenarios, biomass deployment based on optimal system costs is in conflict with the technical GHG abatement potential (i.e. optimal GHG abatement). Prioritizing the technical side over the cost optimal side of GHG abatement could result in additional GHG abatement equivalent to the annual average GHG abatement in the cost optimal objective. The additional GHG savings could be captured at opportunity costs of €779/t CO_2-eq for the base scenario and €1230/t CO_2-eq for the biochemicals deployment scenario.

In the base scenario, the conflict in biomass allocation between the two objective functions stems from SNG, which, in addition to biomethane, is competitive in the GHG abatement objective. In the cost optimal objective, biomethane and bioethanol are competitive. On the other hand, for the biochemicals deployment scenario, the conflict is a result of the production of bioethylene instead of biomethane in the transport sector.

3.4. Best compromise GHG abatement

The technological GHG abatement developments at the best compromise point (i.e. grid point number 14) are shown in Figure 9. In the base scenario, GHG abatement grows from 37 million tonnes in 2020 to 61 million tonnes in 2050, representing a 5.4% GHG emission reduction by 2050 compared to

1990 GHG emission levels in the energy, building, transport and industrial sectors. In the biochemicals deployment scenario, GHG abatement grows from 37 million tonnes to 66 million tonnes, representing a 6% reduction by 2050 compared to 1990 GHG emission levels. The cumulative GHG abatement increases by 8.1% in the biochemicals deployment scenario.

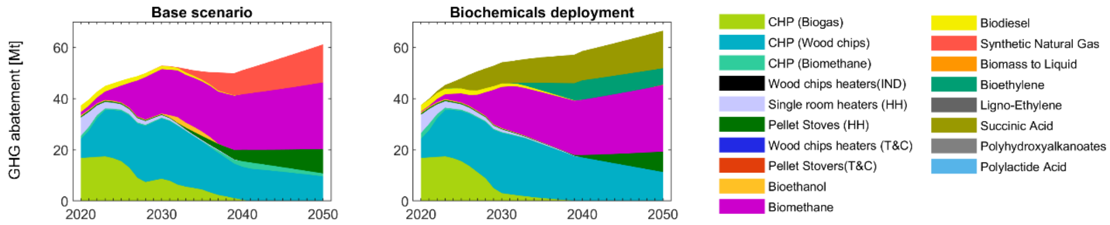

Figure 9: GHG abatement in the tradeoff options in the base and biochemicals deployment scenarios. Here CHP stands for combined heat and power plant, IND for industry, HH for household, and T&C for trade and commerce.

3.5. Biochemicals GHG emissions reductions

As a result of a 1.8% annual increase in the demand for fossil-based ethylene and adipic acid, the latter of which is used in the manufacture of polyurethanes, GHG emissions from the production of these chemicals would increase by 10 million tonnes by 2050. This increase occurs despite the reduction of GHG emissions from electricity (i.e. as a result of the decommissioning of coal power plants), which is used as a utility, suggesting that heat is a major contributor to GHG emissions through the production of these chemicals. The results of the best compromise solution between the cost-optimal and GHG abatement optimal objective functions show that the production of fossil-based ethylene and adipic acid could become GHG neutral by 2050 (see Figure 10). The production of the biochemicals ethylene and succinic acid in 2050 is just less than half of the total demand but this is enough to ensure GHG neutrality even when the other half is met by fossil counterparts. Emission reductions from ethylene production also cover emission reductions for other base chemicals such as propylene, butadiene and aromatics because the GHG emission factor for fossil-based ethylene includes emissions for other products from steam cracking (Neelis et al. 2003). This means that the production of bioethylene and succinic acid could offset emissions even when the demand for propylene, butadiene and aromatics is met by fossil production. Therefore, additional efforts are needed for GHG emission reductions in other subsectors of base chemicals, such as ammonia and methanol. These efforts could include renewable heat, while continuing production from fossil resources or the production of these chemicals from renewable hydrogen and biogenic carbon.

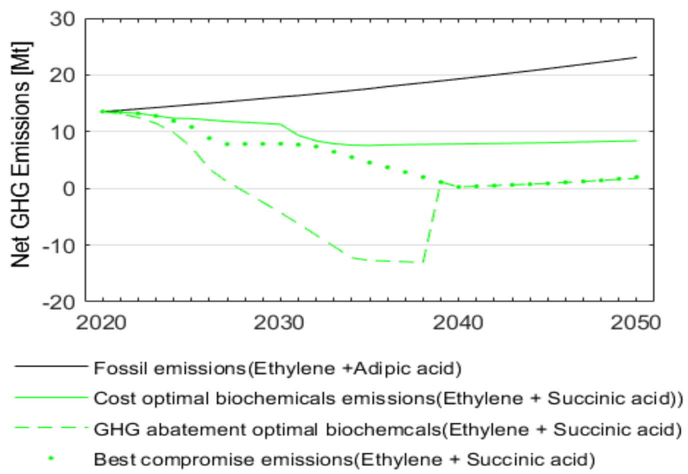

Figure 10: GHG emission reductions from the ethylene and adipic acid subsectors

3.6. Sensitivity analysis of crude oil price developments

In the low crude oil price development, biofuels, biodiesel, BtL and all biochemicals are not cost competitive. In a high crude oil price development, all bio-products are cost competitive except for lignocellulose-based ethylene. The development of the price for natural gas, which has an effect on the cost of woodchips and wood pellets, does not considerably change the cost competitiveness of technologies in the power and heat sectors. CHP plants with woodchips as energy sources, industrial heaters (using woodchips), and single room heaters for households are cost competitive throughout all crude oil price trajectories. On the other hand, pellet stoves and woodchip heaters were found to be competitive in the long term (Appendices D and E).

4. Practical implications of the present study

The technical GHG abatement for bioethylene can, to some extent, be practically implemented under the reference crude oil price scenario because from the results, bioethylene profitability has hovered around zero for some years. This can be stated with certainty for succinic acid because it is a cost competitive option under a reference crude oil price development. However, as a result of the uncertainty regarding how the price for crude oil could develop in the future and how this affects the competitiveness of the identified biochemicals, it is imperative that long-term support mechanisms are formulated to boost uptake in the biochemicals market. One such mechanism could be the introduction of the acquisition of CO_2 emission rights by fossil-based ethylene and adipic acid producers from biochemical producers. In this case, fossil ethylene and adipic acid producers could be mandated to source 40% of bioethylene and succinic acid in order to meet demand. This is because, out of the total theoretical GHG emissions from the production of fossil chemicals (i.e. ethylene and adipic acid), a production allowance of 40% from biochemicals by 2050 could offset the emissions from 60% fossil chemicals because these biochemicals sequester biogenic CO_2 in the final product.

Another support mechanism could be the internalization of carbon dioxide emission externalities by taxing fossil references based on the price of carbon dioxide. A traditional economic approach to determining this is to regard carbon dioxide as a tradable commodity. Its price would then be determined at a point where the marginal social benefit of CO_2 abatement is equal to the marginal social cost of abatement. However, there is no consensus regarding this methodology because of the uncertainty tied to determining how much society is willing to pay to avoid the effects of climate change. Pollitt (2018) argues that this methodology is actually redundant for informing policy because the comprehensive framework for policy makers is based on implementing policies that aim to reduce emissions consistent with the agreement to limit the rise in temperatures to below 2°C in the Paris Agreement. Therefore, in the German context, fossil chemicals could be taxed at the CO_2 price calculated based on the carbon budgets up until 2050 in accordance with the Climate Action Plan.

Thirdly, regulatory policies in the form of chemical standards to facilitate biochemical production quotas, could be effective in stimulating demand, thereby accelerating the market uptake of the studied biochemicals. However, in order to prevent the possibility of carbon leakage and to avoid creating unfair market conditions for the German chemicals industry, the exact biochemical production quota and the general design of the mandate need to be thoroughly studied. The possibility of carbon leakage stresses the need for a unified approach to tackling climate change.

It should be noted that while these measures could support the uptake of biochemicals, the underlying assumption is that there are no market imperfections. In the real world, however, market imperfections, such as farmer and consumer preferences, do exist.

In addition to measures that support the market uptake of biochemicals, targeted measures should be implemented to ensure that carbon dioxide absorbed during the cultivation of biochemical feedstocks is never released at its end of life. This could be done by making plastic waste recycling an attractive business model, firstly by incentivizing the eco-design of the final products, which together with improved sorting at the disposal site, would reduce variability in the physical and chemical characteristics of plastic waste and ensure high-quality recyclates. Secondly, the incineration of plastic waste should be discouraged by taxing energy recovery from plastic waste. Our study shows that the theoretically possible GHG abatement decreases to 4.3% when Germany's current recycling rate of 50% (Coppola 2019) is taken into consideration.

5. Conclusions and future directions of research

In this paper, a bi-objective biomass deployment model is used that has GHG abatement (representing the technical GHG abatement potential) and optimal cost (representing the economically feasible GHG abatement) objectives. Bi-objective optimization facilitates the basis for a more holistic assessment by simultaneously investigating two objective functions, thereby providing an additional perspective for decision making due to the possibility of analyzing best compromise solutions between conflicting objectives.

The potential for additional GHG abatement beyond the energy system as a result of optimal biochemicals deployment in Germany has been calculated to be 8.3% more for the cost-optimal objective and 8.6% more for the GHG abatement-optimal objective. The implication of biochemicals deployment with regard to the status quo is that arable land is preferably used for the cultivation of feedstocks for succinic acid and bioethylene production rather than feedstocks for SNG and biogas/biomethane CHP plants.

Conflicts between the allocation of biomass based on cost and GHG abatement do exist. Additional GHG abatement, which can be achieved from the technical potential (i.e. optimal GHG abatement) relative to the cost-optimal potential, has been quantified and is equivalent to the annual average GHG abatement in the cost-optimal objective. This technical potential for GHG abatement could be achieved without implementation challenges because the technologies that result in the additional GHG savings (i.e. SNG and bioethylene) are economically feasible at the reference crude oil price.

From the best compromise solutions of the cost and GHG abatement optimal objectives (i.e. points where the gradients for the Pareto fronts increase sharply towards the optimal GHG abatement value), the considered biomass potentials in Germany could abate 61 million tonnes of CO_2-eq by 2050, representing a 5.4% reduction in GHG emissions compared to 1990 GHG emission levels in the energy, building, transport and industrial sectors. With the deployment of biochemicals, however, 66 million tonnes of CO_2-eq, representing a 6% reduction by 2050 over 1990 GHG emission levels, could be achieved for the same biomass potentials. Cumulative GHG abatement increases from 1.58 billion tonnes of CO_2-eq in the base scenario to 1.72 billion tonnes (i.e. 8.5% more) in the biochemicals deployment scenario. This comes at reduced biomass usage in the power, heat and transport sectors and increased opportunity costs as a result of the production of bioethylene instead of biomethane, which has a superior economic performance. Furthermore, the production of bioethylene and succinic acid– meeting just 40% of demand– could ensure that the production of fossil ethylene and adipic acid is climate neutral. This is because bioethylene and succinic acid sequester biogenic CO_2 in the end products, thereby resulting in negative emissions.

This result is, however, sensitive to the underlying assumption about the development of the crude oil price. When a lower crude oil price development scenario is taken into consideration, bioethylene and succinic acid are not economically feasible and hence do not play a key role in GHG abatement. A low price development trajectory for crude oil could, therefore, deter the deployment of biochemicals in the German bioeconomy. Additionally, the results are also sensitive to the assumptions regarding the biochemical product's end of life treatment. The generated results are based on the 100% end-of-life recycling of biochemical end products (i.e. no energy recovery). Based on the status quo, however (i.e. 50% recycling rate for plastics in Germany), the additional GHG abatement beyond the German energy system decreases from 8.1% to 4.3% because bioethylene is no longer competitive without ensuring carbon sequestration. Therefore, the end-of-life recycling of biochemical end products is pertinent for GHG abatement in the bioeconomy.

Ambitious renewable energy targets in Germany by 2050 could provoke a decoupling of chemical prices from the crude oil price because, in a fully renewable future, the crude oil price is irrelevant. For future research, it would therefore be interesting to couple the current model with a Computable General Equilibrium (CGE) model in order to bridge this uncertainty. Additionally, as interest in renewable hydrogen in Germany increases, a comprehensive representation of the system could be done by incorporating electro-fuels and electro-chemicals from the electricity grid and/or excess electricity, which is currently being discussed as an important aspect of the German energy transition.

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Appendix A: Life cycle inventory data for biofuels and biochemicals adapted from (Millinger et al. 2017; Majer et al. 2016; Meisel et al. 2016; Jungbluth et al. 2007; Liptow and Tillman 2009; Groot and Borén 2010; Moussa et al. 2016; Zhong et al. 2009). In the table, EthOH stands for ethanol, $BioCH_4$ for biomethane, RME for biodiesel, SNG for synthetic natural gas, BtL for biomass to liquid, PHA for polyhydroxyalkanoates and PLA for polylactic acid. The units for conversion efficiency are GJ/tFM for biofuels and t/tFM for biochemicals and the values are based on (Ponitka et al. 2015; Liptow and Tillman 2009; IfBB 2017).

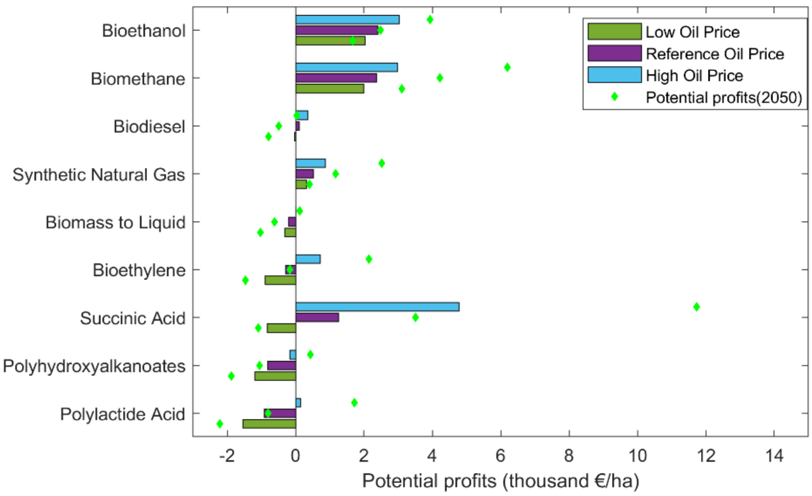
	Units	**EthOH**	**BioCH4**	**RME**	**SNG**	**BtL**	**Bio_Ethylene**	**Ligno-ethylene**	**Succinic**	**PHA**	**PLA**
Feedstock		Sugar beet	Maize silage	Rapeseed	Poplar	Poplar	Sugar beet	Forest biomass	Corn	Corn	Corn
Yield_2015	tFM/ha	65	45	3.5	18	18	65		9.3	9.3	9.3
Yield_2050	tFM/ha	65	55	3.5	27	27	65		9.3	9.3	9.3
P2O5	kg/ha	59.7	38.5	33.7	34.35	34.35	59.7		54.5	54.5	54.5
K2O	kg/ha	134.9	24	49.5	55.2	55.2	134.9		67	67	67
Insecticides	kg/ha	1.3	7	1.2			1.3		0.6	0.6	0.6
CaO	kg/ha	400	1000	19	103.6	103.6	400		283	283	283
MgO	kg/ha				18.26	18.26					
N2O including field N_2O emissions	kg/ha	3.27	4.66	3.1	1.28	1.28	3.27		4.66	4.66	4.66
N	kg/ha	119.7	63.2	137.4	0	0	119.7		106.5	106.5	106
Seeds	kg/ha	6	25	6	0	0	6		30	30	30
Diesel	L/ha	175.9	96	82.6	2.1	2.1	175.9		55	55	55
Electricity	kWh/ha			70.3							
Carbon sequestration	kg CO_2/tFM						308		1258		
Processing											
Conversion efficiency	GJ/tFM or t/tFM	2.3	3.3	14	4.6	2.8	0.05	0.1	0.4	0.2	0.3
Heat	MJ/t feed	1131.2	778.8	1133.7			1381.2	585	819	1804	5266
Electricity	kWh/t feed	29.9	46.6	22.9	142.2	97.02	72	219.2	1477	1015	1286

Appendix B: Parameters used to calculate life cycle costs for bioenergy and biofuels. In the table, P-H stands for power and heat sectors, H (IND) for the industry subsector of the heat sector, H (HH) for the household subsector of the heat sector, and H (T&C) for the trade and commerce subsector of the heat sector. CHP_Biogas stands for CHP plants using biogas, CHP_WC for CHP plants using woodchips, CHP_CH_4 for CHP plants using biomethane, Heater_WC for heaters using woodchips, PS for pellet stoves, EthOH for ethanol, $BioCH_4$ for biomethane, RME for biodiesel, SNG for synthetic natural gas and BtL for biomass to liquid.

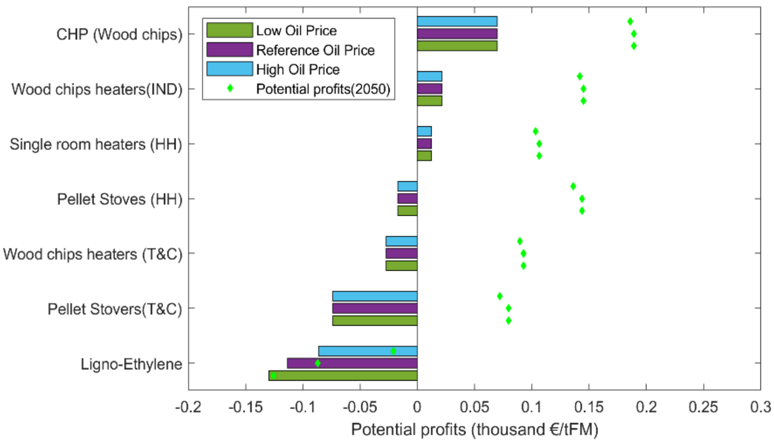
	Units	CHP_Biogas	CHP_WC	CHP_CH_4	Heater_WC	SRH	PS	Heater_WC	PS	EthOH	$BioCH_4$	RME	SNG	BtL
Sector		**P-H**	**P-H**	**P-H**	**H (IND)**	**H (HH)**	**H (HH)**	**H (T&C)**	**H (T&C)**	**Transport**	**Transport**	**Transport**	**Transport**	**Transport**
Capital costs	€/kW	5250	4300	4500	195	200	100	1500	1250	800	1700	245	3500	3850
O&M without feed costs	% of investment	3.9	10.3	3.3	25.7	6	6	10.3	7.7	6.6	5.9	7.8	4.2	2.5
Base capacities	GW	6.7	1.51	0.78	6.1	115	5.6	6	0.7	1.05	0.71	6.18	0	0
Plant life	y	20	20	20	20	15	20	20	30	20	20	20	20	20
Product yield 2015	GJ/tFM	1.27	5	1.27	10	8.6	13.26	10	13.26	2.35	3.33	14.23	4.6	2.8
Product yield 2050	GJ/tFM	1.3	5.3	1.3	11.3	9.3	15.3	11.3	15.3	2.6	4.2	15	5.8	3.3

Appendix C: Parameters used to calculate life cycle costs for biochemicals (Vaswani 2010; Roland-Holst et al. 2013; Tides Center/Environmental Health Strategy Center and Maine Initiatives with Jim Lunt & Associates, LLC 2010; IEA-ETSAP and IRENA 2013).

	Units	Bio_Ethylene	Ligno_Ethylene	Succinic acid	Polyhydroxyalkanoates	Polylactic acid
Capital costs	€/t	1291	1291	3643	5667	6184
O&M without feed costs	% of investment costs	6.6	6.6	22.9	14	14
Base capacities	t	0	0	0	0	0.05
Plant life	y	20	20	20	20	20
Product yield 2015	t/tFM	0.046	0.105	0.371	0.19	0.31
Product yield 2050	t/tFM	0.05	0.13	0.414	0.21	0.35



Appendix D: The development of potential profits in euros per hectare (€/ha) for biobased technologies with feedstocks from arable agricultural land. The bars represent the potential profits per hectare of land used for feedstock cultivation in 2020, while the points refer to the potential profits in 2050.



Appendix E: The development of profit in euros per ton of fresh matter (€/tFM) for biobased technologies with feedstocks from forest biomass. The bars represent the potential profits per ton of fresh matter for land used for feedstock cultivation in 2020, while the points refer to the potential profits in 2050. In the figure, CHP stands for combined heat and power plant, IND for industry, HH for household and T&C for trade and commerce.