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Musonda, F., Millinger, M., Thrän, D. (2024). Modelling assessment of resource competition for renewable basic chemicals and the effect of recycling. *GCB Bioenergy*, 16(4). <http://dx.doi.org/10.1111/gcbb.13133>

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RESEARCH ARTICLE

Modelling assessment of resource competition for renewable basic chemicals and the effect of recycling

Frazer Musonda¹ | Markus Millinger² | Daniela Thrän^{1,3}

¹Department of Bioenergy, Helmholtz Centre for Environmental Research–UFZ Permoserstraße 15, Leipzig, Germany

²Department of Space, Earth and Environment, Chalmers University of Technology, Göteborg, Sweden

³DBFZ Deutsches Biomasseforschungszentrum gemeinnützige GmbH, Leipzig, Germany

Correspondence

Frazer Musonda, Department of Bioenergy, Helmholtz Centre for Environmental Research–UFZ Permoserstraße 15, 04318 Leipzig Germany.
Email: frazer.musonda@ufz.de

Funding information

Bundesministerium für Bildung und Forschung, Grant/Award Number: 031B0281A-031B0281II

Abstract

This work assesses pathways towards a net-zero greenhouse gas (GHG) emissions chemical industry sector in Germany until 2050, focusing on the ammonia, methanol, ethylene and adipic acid subsectors and the effect of the recycling of C embedded in chemical end products on the GHG abatement cost and primary resource demand. This was done using a bottom-up mathematical optimization model, including the energy sectors and the chemicals sector, with electricity and biobased options considered. Results show that net-zero GHG emissions for the considered chemicals in 2050 are attainable at a marginal cost of 640–900€/tCO₂-eq, even with 26%–36% of demand being satisfied by fossil production routes. This is possible because renewable organic chemicals can act as carbon sinks if, at their end of life, C is permanently stored via landfilling or passed on to the next value chain via recycling. Nonetheless, considering the cost implications, the practical deployment of renewable chemicals is a challenge. The considered renewable chemicals cost 1.3–8 times more than their fossil counterparts, resulting in a marginal CO₂ price of 480€/tCO₂-eq when all primary resources (energy crops, forest residues and renewable electricity) are considered, or 810€/tCO₂-eq when the availability of arable land is restricted. In the transition to net-zero emissions for the chemicals under study, a circular economy is important not only for reducing demand for primary resources as is typically the case but also reduces GHG abatement costs by 13%–24% through carbon capture and utilization effects.

KEYWORDS

biochemicals, biogenic CO₂, GHG abatement, recycling, renewable chemicals, renewable hydrogen, sector coupling

1 | INTRODUCTION

According to the Inter-governmental Panel on Climate Change (IPCC), anthropogenic greenhouse gas (GHG)

emissions need to be reduced to net zero by 2050 if global warming is to be limited to 1.5°C (IPCC, 2018). The German government, in acknowledging this reality, framed a strategy which laid out the long-term GHG

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emissions reduction development in line with the Paris agreement (BMUB, 2016). Key aspects of Germany's mid-century GHG neutral strategy are the decommissioning of coal power plants and the expansion of wind and solar power generation. The challenges that are associated with the increased deployment of wind and solar energy, such as intermittency (Zsiborács et al., 2019) and possible mismatch with the electricity transmission grid (Deign, 2020) could be solved through sector coupling. Renewable hydrogen (H_2), that is H_2 produced from the electrolysis of water using renewable electricity, is an important element of sector coupling which can be used as an energy storage medium (BMW, 2020), directly or indirectly (i.e. via synthetic fuels) in the transport sector and in the chemicals industry, which are difficult to decarbonize (BMW, 2020). In addition to renewable H_2 , biomass resources are relevant in an increasingly renewable German power sector (Tafarte et al., 2017) and the chemicals sector (Musonda et al., 2021).

There has been growing interest in assessing transformational pathways for the chemicals industry using bottom-up mathematical models in the recent past (Daioglou et al., 2015; Saygin & Gielen, 2021; Tsiropoulos et al., 2017). Daioglou et al. (2015) assessed the potential role of biomass for the energy and chemicals sectors on a global scale until the year 2100. Under baseline conditions, they concluded that 170 EJ/year of secondary bioenergy could be consumed globally in 2100, which translates in approximately 18% of total secondary energy demanded in the transport, heating (i.e. buildings) and chemical sectors. A similar assessment was done by Tsiropoulos et al. (2017) for Netherlands in 2030. In most of the scenarios they considered, the emission reduction targets for the Netherlands were not met, and therefore, they recommended a stronger climate policy as an important determinant for the development of a bioeconomy. Zibunas et al. (2022) calculated CO_2 prices necessary for zero emissions for the chemicals industry in 2050 ranging between 57 and 912 \$/ CO_2 -eq across 'Business as usual', 'Sustainable Development' and 'net-zero emissions' scenarios. On the other hand, Saygin and Gielen (2021) calculated an average value of 64 \$/ CO_2 -eq for full defossilization in 2050 on a global scale in their study which also showed that renewables-based solutions could account for more than half of the total emissions reduction potential if bioenergy with carbon capture and storage (BECCS) is taken into account.

However, in view of the 2050 climate targets for Germany, these studies cannot give concrete insights regarding the role of biomass and renewable H_2 and the corresponding abatement costs. This is mainly due to different temporal scopes, different primary resource potentials, different goals for the evolution of the power

sector (a key assumption for calculating the availability of renewable H_2), different political climates etc. Saygin and Gielen (2021) have partly acknowledged this by mentioning that 'global strategies cannot simply be applied equally at the country/region level without tailoring'.

In the context of Germany, DECHEMA and FutureCamp (2019) have recently assessed possible transformational pathways for the chemicals industry towards net-zero emissions in 2050 whilst incorporating renewable hydrogen and biomass as feedstocks. In their work, the availability of electricity for electrolysis is not restricted by national scenarios that depict capacity expansions for power production in Germany until 2050. Additionally, the competition for primary resources, that is biomass and renewable H_2 , from other competing sectors is not captured. Furthermore, succinic acid which can replace adipic acid, which has a high GHG footprint, and bioethylene, a promising replacement for fossil-based ethylene, were not considered.

The purpose of this work, therefore, is to assess net-zero GHG emissions pathways for some basic chemicals by 2050 in Germany, in order to capture complexities that studies at the global level cannot capture, such as detailed primary resource potentials, final demands evolution, politically set national targets (because not all countries will move at the same pace regarding 2050 targets) and the interaction with the energy system. For this purpose, additionally, the availability of renewable H_2 is regarded to be constrained based on solar and wind power capacity expansion scenarios until 2050. Biobased ethylene and succinic acid are considered in the scenarios for this work.

The use of carbon capture and storage (CCS) for bioenergy has been shown as cost-effective for achieving climate targets (IPCC, 2018), because of the advantage of capturing and permanently storing biogenic CO_2 , thereby resulting in negative emissions. For the chemicals sector, the equivalent for achieving this is the use of CCS during the recovery of energy from chemical end products at their end of life or through chemical recycling. For this work, therefore, the potential role of recycling (in this context meaning chemical recycling) is additionally assessed.

The following questions are sought to be answered:

- What are the cost implications of a net-zero GHG emissions chemicals sector in Germany?
- How does recycling of carbon embedded in products affect the GHG abatement cost of renewable chemicals?

2 | MATERIALS AND METHODS

We base our methodology on scenario/sensitivity analysis on the BioENergy OPTmization model (BENOPT)

(Millinger, Tafarte, et al., 2022). In this work, the chemicals sector is added to the power, heat and transport sectors which are originally in the model. Thus, we can assess the potential contribution of biomass and renewable H₂ resources towards GHG abatement for the considered chemicals in a system representation.

The considered chemicals, ethylene, ammonia and methanol represent a direct replacement to the major basic chemicals because they have the same chemical formula. Succinic acid on the other hand can technically replace fossil adipic acid which has a significant production volume and abatement potential in Germany (Musonda et al., 2020). For the carbon-based chemicals (i.e. all the chemicals except ammonia), the indefinite recycling of their end products at their end of life (i.e. the passing on of C to the next value chain) could ensure that these chemicals have negative emissions (Musonda et al., 2021). As a result of these negative emissions, the fossil references in this work do not necessarily have to be replaced completely to achieve net-zero emissions.

2.1 | The model

BENOPT is a linear optimization model, with the objective of allocating biomass and renewable H₂ to the power, heat and transport sectors in a cost/or GHG abatement optimal manner. The model is bottom-up with perfect foresight and is fully deterministic.

The focus of this work was to assess cost-optimal transformational pathways towards net-zero GHG emissions for the considered chemicals. The optimization is done in 2 steps, the first being based on maximizing GHG abatement and the second is based on minimizing abatement costs with the determined maximal GHG abatement from the first optimization step set as a target (i.e. set as a constraint) for the power, heat and transport sectors. For the chemicals sector, a linear reduction of GHG emissions to zero in 2050 is set as the target.

Exogenous input data such as technology-specific data, resource potentials, etc. and scenario-specific data/restrictions are imported from an Excel spreadsheet through MATLAB where some pre-calculations, such as annualized investment costs, feedstocks price development and life cycle GHG emissions, are done and the data is transferred to the main model in GAMS for optimization. Based on this data, the model allocates the limited resources, that is biomass and H₂, to competing uses in the power, heat, transport and chemicals sectors based on minimizing costs while being constrained by capacity expansion, primary resource availability, the GHG target and sectoral upper demands. Details for the

objective functions and the constraints is supplied in the 'Supporting Information'.

2.2 | Considered renewable chemicals

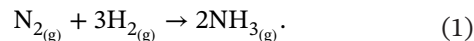
Figure 1 shows the main raw materials for the petrochemicals industry, the conversion steps for producing basic chemicals and the downstream products from the basic chemicals. The fundamental processes to produce basic chemicals are;

- (i) Catalytic reforming of naphtha (yielding basic chemicals xylene, toluene and benzene).
- (ii) Steam cracking of naphtha (yielding ethylene, propylene and butadienes).
- (iii) Production of syngas via steam reforming of methane (for methanol production).
- (iv) Haber-Bosch process yielding ammonia.

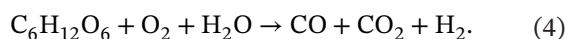
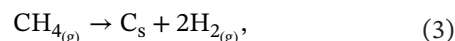
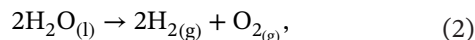
For the modelling in this work, the renewable chemicals considered that can technically replace some of the fossil chemicals are:

2.2.1 | Ammonia

Ammonia, a base chemical for the production of all nitrogen fertilizers which are important for agriculture, is produced from the reaction of H₂ and Nitrogen (N₂) (Equation 1). From Figure 1, ammonia is the only non-C-containing basic chemical and is referred to as an '*inorganic chemical*'. Carbon-containing basic chemicals are referred to as organic chemicals.



In the model, the H₂ for this reaction is produced from the electrolysis of water (Equation 2), from the pyrolysis of biomethane (Equation 3) and from the gasification of biomass residues (Equation 4).



2.2.2 | Methanol

Methanol is either produced via the hydrogenation of captured biogenic CO₂ (Equation 5) or via the reaction of syngas (i.e. product mixture of CO and H₂ produced

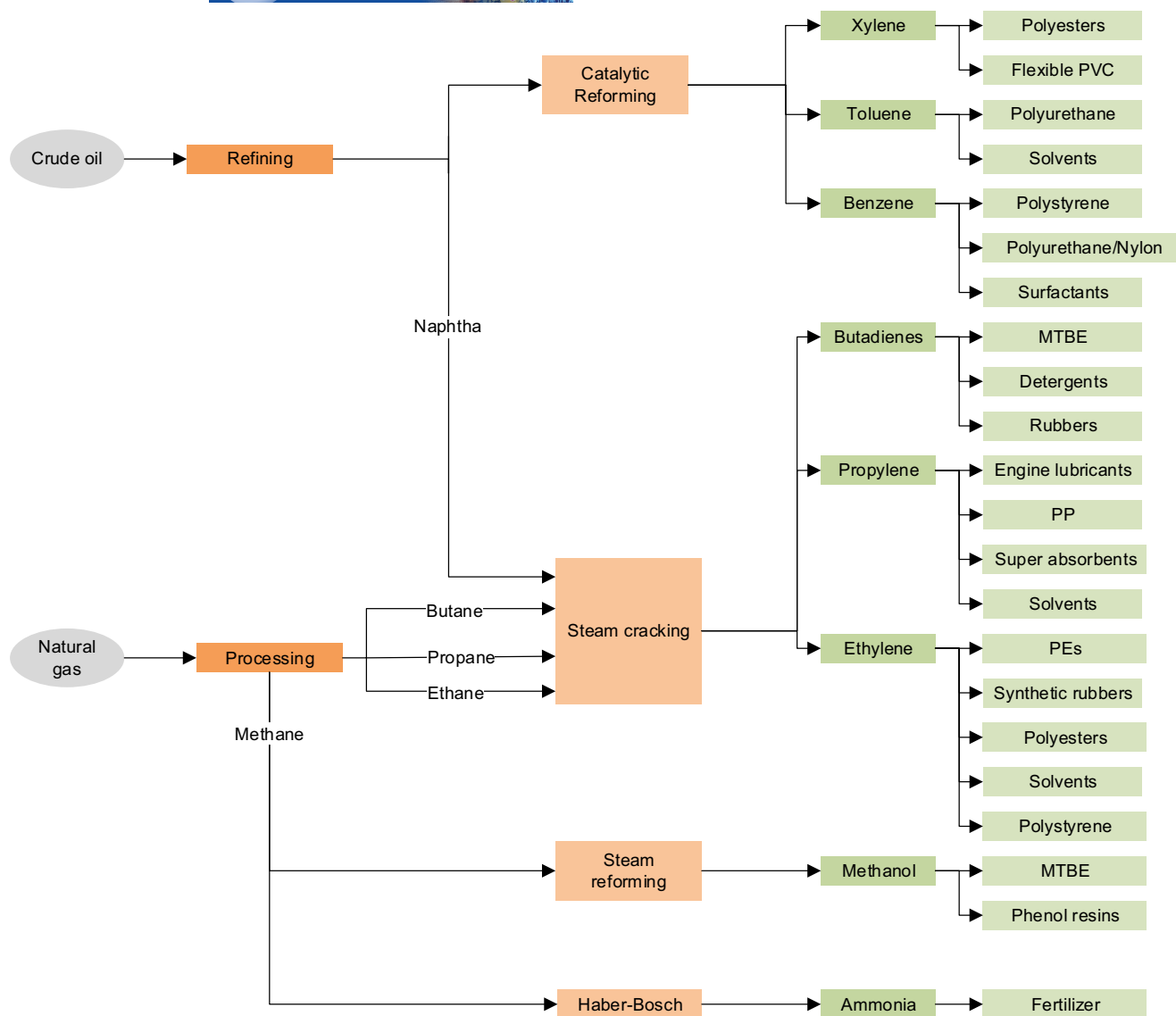
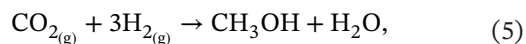


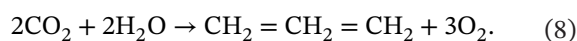
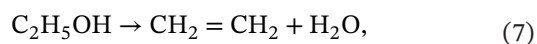
FIGURE 1 Fossil-based value chains from feedstocks, processing steps for production of basic chemicals, intermediate chemicals and final products.

from the gasification of biomass) using a catalyst (Equation 6). The H_2 in Equation (5) is derived as in Equations (2–4).



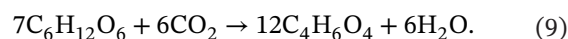
2.2.3 | Ethylene

Ethylene is either produced from the catalytic dehydration of bioethanol (Equation 7) or from the electrochemical reduction of captured biogenic CO_2 (Equation 8)



2.2.4 | Succinic acid

Succinic acid is produced from the anaerobic fermentation of glucose (Equation 9)



In Figure 2, the modelling framework showing the renewable chemicals value chains is shown. Renewable ethylene, methanol and ammonia are drop-in chemicals (i.e. renewable chemicals with the same chemical structure and properties as their fossil references) that can

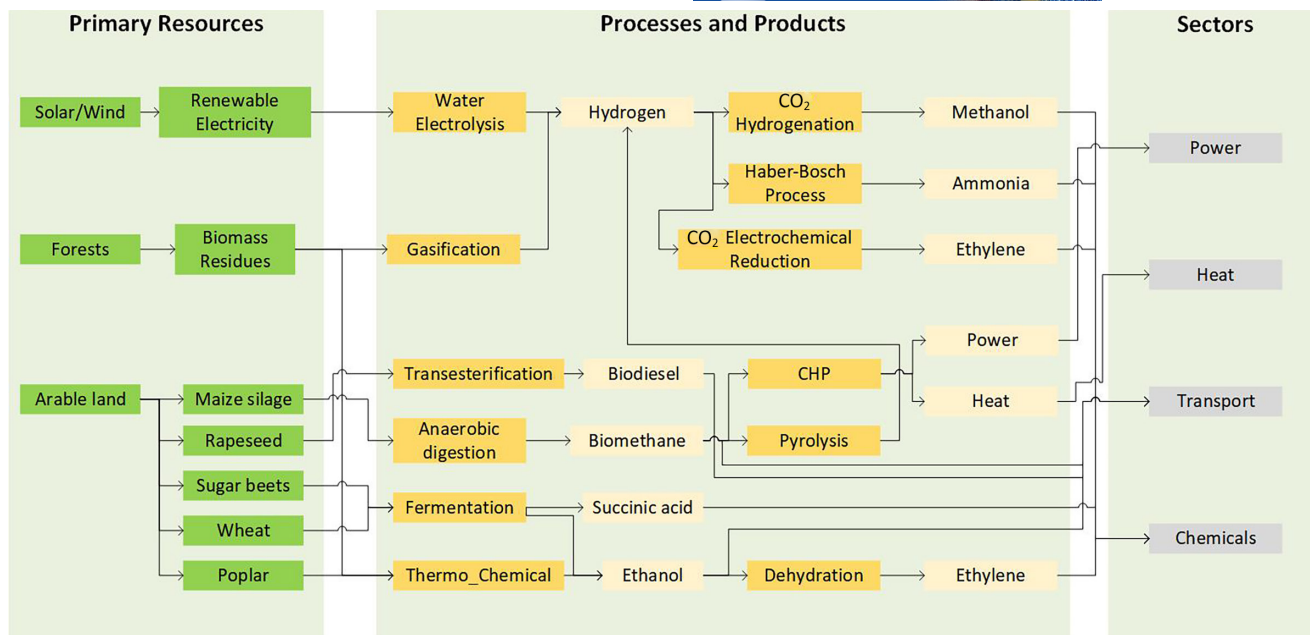


FIGURE 2 Modelling framework with renewable chemicals value chains.

directly replace basic chemicals produced from processes (ii), (iii) and (iv), respectively. For process (ii), renewable references for butadienes and propylene (which are normally produced in lesser quantities than ethylene) could not be established from literature. However, the emission factor for fossil ethylene considered in this work is a combination of all products from steam cracking of naphtha. Therefore, all emissions from this fossil process step are accounted for. For process (i), renewable references were not established for all the fossil basic chemicals. To account for some emissions from this subsector, however, adipic acid, which is used to produce polyurethanes (which are produced in large quantities in Germany) was modelled with succinic acid as a renewable replacement.

2.3 | Data and assumptions

2.3.1 | Life cycle costs

The life cycle costs for the considered renewable chemicals include costs for the feedstocks, costs for utilities such as heat and power, fixed operation and maintenance costs, and the costs for capital investments. For ammonia (derived from renewable H_2) and methanol (derived from renewable H_2 and forest residues) all data regarding investment, and fixed operation and maintenance costs is based on (DECHEMA & FutureCamp, 2019). For ethylene and succinic acid, however, these data are based on (IEA-ETSAP & IRENA, 2013; Vaswani, 2010). Table S1 A summarizes this data.

The assumptions for the price of heat and power, which contribute to the variable operation and maintenance costs

is based on (Thrän et al., 2019). On the other hand, the price development for excess electricity is based on the electricity price according to (DECHEMA & FutureCamp, 2019). The development of energy crop prices over the temporal scope is based on a methodology in which the profit from wheat (i.e. benchmark crop for Germany) production per hectare is added to the per hectare production costs of the considered energy crops. A detailed explanation for this methodology can be found in (Millinger & Thrän, 2018).

2.3.2 | Life cycle GHG emissions

The total emissions for each renewable chemical are based on the sum of emissions from the cultivation of feedstocks or the production of renewable hydrogen and the emissions throughout all the conversion processes up to the final product. Emissions based on these values are calculated by multiplication with specific emission factors. This information is summarized in Table S2.

For the temporal scope in our study, the German power grid emission factors are based on a scenario development from (WWF, 2017) in which coal power plants are supposed to decommission after a plant lifetime of 20 years and in which there is an ambitious expansion of renewable energies.

2.3.3 | German power sector development

In this work, the development of capacities for solar PVs, onshore and offshore wind and the corresponding

load hours is based on (BWE, 2020a, 2020b; Henning & Palzer, 2013; Millinger et al., 2021; Rohrig et al., 2014; Wirth, 2020). Values for 2030 are based on the new EEG amendment (BMWK, 2023) which are interpolated to 2050. This is summarized in Table 1.

2.4 | Organic chemicals carbon storage

Except for ammonia, which is an inorganic basic chemical used for the production of all nitrogenous fertilizers, the organic basic chemicals (i.e. chemicals containing carbon) considered in this work are used for the production of a variety of chemicals/products which find applications in a wide range of sectors. Polymers and plastics which constitute 80% of the worldwide chemical industry's output (Boyle, 2022), are used to make electric and electronic appliances, automotive parts, construction and building materials, footwear, sports equipment, textile, thermal insulation materials, home furnishings, food packaging etc. (Petrochemicals Europe, 2023). The remaining organic chemicals are used as coolants, lubricants, solvents, adhesives, paints, coatings, inks etc. At their end of life, which varies from less than a year to over 80 years, organic chemical end products can in theory be reused, recycled and landfilled, or incinerated. The status quo on the global scale is that 50% of the plastic waste is landfilled, 22% is mismanaged, 19% is incinerated for energy recovery while 9% is recycled (OECD, 2022). In the context of renewable plastics, this statistic hypothetically implies that over 60% of renewable C contained in plastic wastes could be permanently stored in the products (i.e. via landfilling) or is passed on to the next value chain (i.e. via recycling). In the context of Germany where the recycling rate is 50% (Coppola, 2019) and the rest goes to incineration for energy recovery, 50% of renewable C could be stored by being passed to the next value chain. Therefore, provided that the production-based GHG emissions are less than the CO₂ uptake, this would result in negative emissions. Elemental carbon in organic compounds can only be

TABLE 1 Solar and wind power plant installation capacities (GW, gigawatt) and full load hours (FLH, kWh kW⁻¹) development assumptions (BMWK, 2023; BWE, 2020a, 2020b; Henning & Palzer, 2013; Rohrig et al., 2014; Wirth, 2020; WWF, 2017).

	Solar PV	Onshore wind	Offshore wind
GW2020	49	54	7.5
GW2050	677	325	80
FLH2020	935	2000	4091
FLH2050	951	2295	4290

released as CO₂ through combustion and microbial decay (with the aid of bacteria), the latter process not being possible for plastics derived from the chemicals in this study because they are not biodegradable.

2.5 | Scenarios

The availability of primary resources, that is, the future potential for biomass and excess renewable H₂, is uncertain because it depends on multiple factors such as climate change, climate policies, energy demand, changing diets, population growth etc. As a result of these uncertainties, it is important to assess the future range of possibilities with a scenario approach. Therefore, 3 scenarios for the availability of these primary resources for the modeling have been considered. Millinger et al. (2019) calculated 1.5 Mha of agricultural land for the cultivation of energy crops for biofuels production in Germany. In this work, for scenarios in which energy crops are allowed in the model, an agricultural land of 1.5 Mha is given as this presents a more conservative assumption. In the 'Bio+H₂' scenario, all the primary resources, that is arable land, forest residues (300PJ, Lauer et al., 2023) and renewable H₂ from excess electricity are considered. In the 'ZeroH₂' scenario renewable H₂ is not considered for the assessment while arable land (1.5 Mha) and forest residues (300PJ) are considered. In the 'ZeroLand' the available arable land linearly decreases from 1.5 Mha in 2020 to zero in 2050. An upper value of 300 PJ in 2050 for forest residues is considered. Chemicals production was rather constant during 2010–2020 (VCI, 2018, 2021), and therefore, we assume constant upper sectoral demands for the considered chemicals until 2050 in all scenarios, as shown in Table S5.

The three scenarios are simultaneously assessed with a 'Low' and 'High' level of C recycling, resulting in 6 scenarios in total. With the 'Low' level of recycling, our work attempts to mimic the status quo regarding the level of recycling in Germany (i.e. 50%) (Coppola, 2019) while the 'High' level of C recycling assumption (i.e. 80%), we show how an ambitious strategy for recycling and/or energy recovery coupled with CCU could impact net-zero emissions. In all the considered scenarios, a linear reduction from the status quo GHG emissions to zero CO₂ emissions by 2050 is considered as a target. The considered scenarios are summarized in Table 2.

2.6 | Sensitivity analysis

A sensitivity analysis was performed to assess the effect of input parameter uncertainty on the GHG abatement cost of the renewable chemicals. Firstly, this is done by Monte

TABLE 2 Scenario description.

Scenario	Arable land	Forest residues	Renewable hydrogen from excess electricity
Bio + H ₂	1.5 Mha	300PJ	Yes
NoH ₂	1.5 Mha	300PJ	No
ZeroLand	0	300PJ	Yes

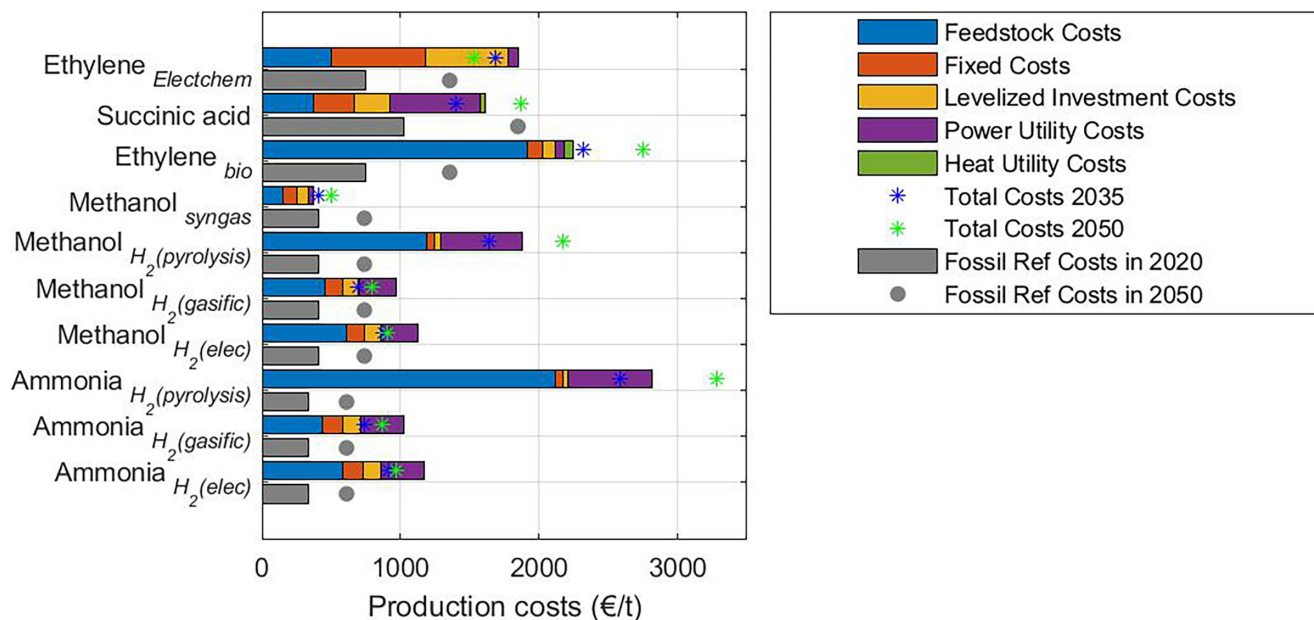


FIGURE 3 Cost components for the considered renewable chemicals for 2020 and the development of total costs until 2050. Ammonia_{H₂(elec)} and methanol_{H₂(elec)} represent ammonia and methanol produced using renewable H₂ derived from the electrolysis of water while ammonia_{H₂(pyrolysis)} and methanol_{H₂(pyrolysis)} represent ammonia and methanol produced using H₂ from biomethane pyrolysis. Ammonia_{H₂(gasific)} and methanol_{H₂(gasific)} represent ammonia and methanol produced using H₂ from the gasification of biomass. Methanol_{syngas} is methanol produced from syngas which is derived from the gasification of biomass residues. The value for the cost of the fossil reference for succinic acid is based on the difference of the current selling price for adipic acid (ECHEMI, 2021) and the average profit (based on the average margin for the chemicals industry in Germany, Utsch, 2015). This approach was undertaken because the production costs could not be established from literature.

Carlo simulations to determine the overall uncertainty of the model, and secondly by multiple linear regression analysis, to identify the contribution of input parameters to the overall uncertainty. 1200 Monte Carlo runs were performed with random parameter combinations from the specified input parameter ranges. The multiple linear regression was done in a Python script with uncertain input parameters as independent variables and the GHG abatement cost as the dependent variable. In Table S6 uncertain input parameters of interest in the model are shown together with the range of variation.

3 | RESULTS

Using the preceding described methodology, key findings for the cost implications of net-zero GHG emissions by 2050 and the effect of the recycling of chemical end products at their end of life, emerge;

3.1 | Net-zero GHG emissions cost implications

In Figure 3, the cost components for the renewable chemicals in the base year (i.e. 2020) and total costs in the years 2035 and 2050, as well as production costs of the fossil references for 2020 and 2050 are presented. Generally, feedstock costs contribute the most to the total cost of all the renewable chemicals, with ammonia produced via the pyrolysis of biomethane, having the highest feedstock cost contribution per total cost. Ammonia and methanol, both produced from renewable H₂ via the pyrolysis of biomethane and ethylene have the highest cost difference with their fossil references while methanol produced via gasification of biomass has the lowest.

Based on the highlighted cost differences (as shown in Figure 3) and the GHG emissions for the fossil reference, the carbon prices needed as a tax instrument on fossil

references for the competitive renewable technologies are calculated for the year 2050 (see Table 3). The CO₂ prices range between 0 and 810€/tCO₂e_q across the considered scenarios.

Figure 4 shows the GHG emissions for the renewable chemicals differentiated by emissions from feedstocks cultivation and energy emissions from production processes. Renewable chemicals whose feedstocks have biological origins generally have the highest GHG emissions stemming from feedstocks cultivation. Overall, the net emissions for the renewable chemicals are better than their fossil counterparts. This would still be the case even when biogenic C storage is not considered because the fossil references emission factors do not include the carbon embedded in the product and the biogenic CO₂ released would be considered neutral. Fossil reference emission factors are generally based on emissions which the industry has control

TABLE 3 CO₂ costs (in €/tCO₂-eq) in 2050 for the competitive technologies.

Ammonia _{H₂(elec)}	170
Ammonia _{H₂(gasific)}	121
Methanol _{H₂(elec)}	161
Methanol _{H₂(gasific)}	60
Methanol _{syngas}	0
Ethylene _{bio}	480
Ethylene _{Lignocellulose}	810
Succinic acid	0
Ethylene _{Electchem}	102

over (TfS, 2022) and do not focus on the end-of-life emissions for the chemicals.

In Figure 5, the GHG abatement costs and the corresponding potential GHG abatement associated with a net-zero emissions target in 2050 for the considered renewable chemicals are shown. Generally, across all the considered scenarios, ammonia_{H₂(elec)} (i.e. produced from hydrogen derived from electrolysis of water) and methanol (i.e. produced from syngas from hydrogen derived from electrolysis of water) have the lowest GHG abatement costs. In scenario Bio + H₂, with the low recycling rate assumption, representative of the status quo for the recycling of end products at their end of life, ammonia_{H₂(elec)} has the lowest GHG abatement cost of 460€/tCO₂-eq while methanol_{elec} (i.e. produced from hydrogen derived from electrolysis of water) is the marginal GHG abatement with a cost of 715€/tCO₂-eq. In the ZeroH₂ scenario, the marginal GHG abatement cost is 682€/tCO₂-eq from ethylene. As can be seen from the ZeroH₂ scenario, ammonia produced using renewable hydrogen from the gasification of biomass has a higher GHG abatement cost (23%) than ammonia produced using hydrogen from the electrolysis of water. A notable difference in abatement costs between the ZeroLand scenario and the Bio + H₂ and ZeroH₂ scenarios is the increase in the abatement cost for bioethylene (i.e. 34%), which can be explained by the fact that the bioethanol used is from lignocellulose biomass rather than sugar beets or wheat.

With a higher rate of recycling, compared to the status quo, the cost of GHG abatement per ton CO₂e_q is lower for ethylene, methanol and succinic acid. This is because

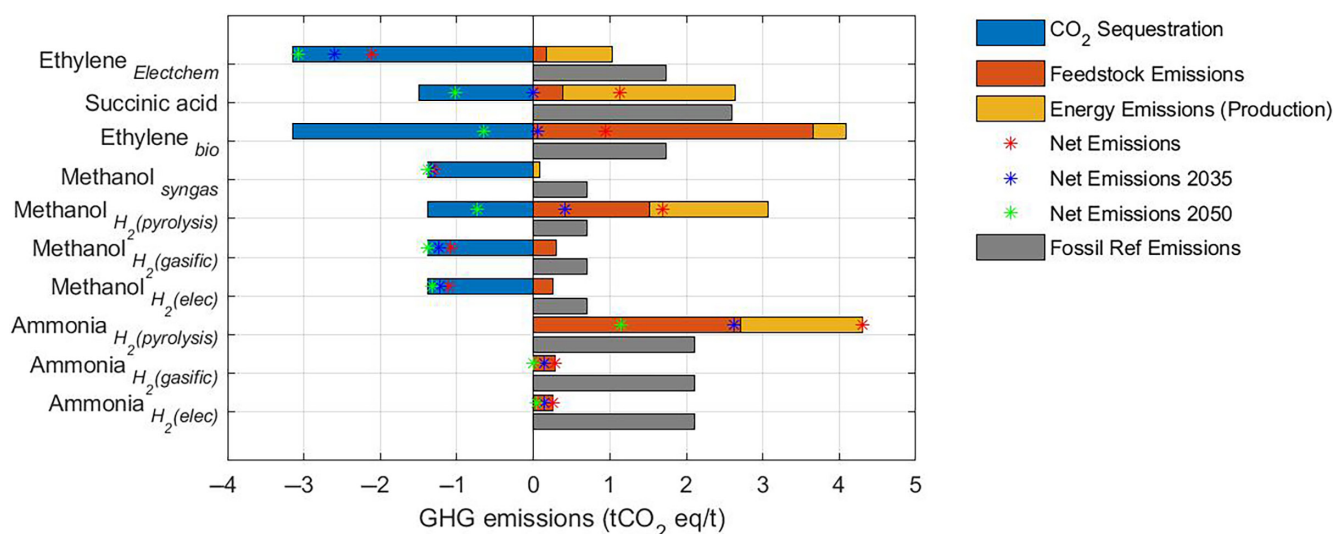


FIGURE 4 The greenhouse gas (GHG) emissions for the considered renewable chemicals for 2020 and the development of the total emissions until 2050. Ammonia_{H₂(elec)} and methanol_{H₂(elec)} represent ammonia and methanol produced using renewable H₂ derived from the electrolysis of water while ammonia_{H₂(pyrolysis)} and methanol_{H₂(pyrolysis)} represent ammonia and methanol produced using H₂ from biomethane pyrolysis. Ammonia_{H₂(gasific)} and methanol_{H₂(gasific)} represent ammonia and methanol produced using H₂ from the gasification of biomass. Methanol_{syngas} is methanol produced from syngas which is derived from the gasification of biomass residues.

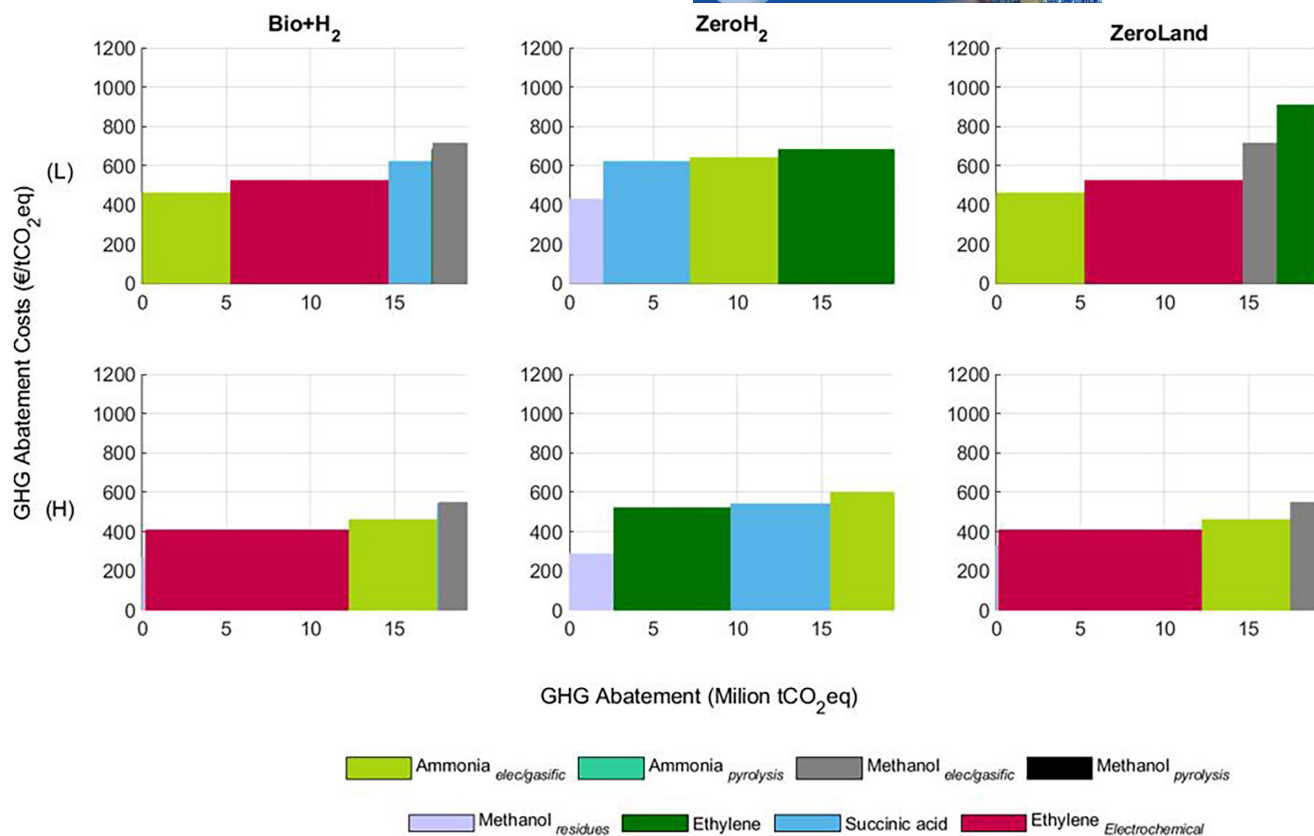


FIGURE 5 Marginal abatement cost curves for the year 2050 in the considered scenarios. Bio + H₂ is the scenario in which all primary resources are considered, in ZeroH₂, renewable H₂ from the electrolysis of water and ZeroLand, agricultural land linearly reduces to zero in 2050. (L) assumption of low recycling rates (50%), (H) assumption of high recycling rates (80%). Ammonia_{H₂(elec/gasific)} and methanol_{H₂(elec/gasific)} represent ammonia and methanol produced using renewable H₂ derived from the electrolysis of water and biomass gasification. Methanol_{syngas} is methanol produced from syngas produced from biomass gasification. Ethylene_{Electchem} is ethylene produced via the electrochemical reduction of captured biogenic CO₂.

the production of these chemicals takes up biogenic C in the form of CO₂ at some point in their production chain and storage of C in chemical products made possible by recycling of their end products at their end of life and storage of CO₂ using CCS when chemical end products are incinerated for energy recovery at their end of life, ensures that this biogenic C is not released in the form of CO₂. Therefore, as a result of higher C recycling, which results in negative emissions, GHG abatement costs for succinic acid and ethylene reduce by 13% and 24%, respectively. The lower reduction in abatement costs for succinic acid relative to ethylene, considering that the increase in the rate of C recycling is the same, can be explained by the fact that succinic acid has a higher GHG emission fossil reference than ethylene.

3.2 | Primary resource demands

In Figure 6, the demand for primary resources needed for net-zero emissions in 2050 for the considered chemicals

in the different scenarios is shown. GHG emissions for the chemicals sector are modelled to reduce linearly from current emissions (2020) to zero in 2050. As a result, fossil chemicals do not necessarily need to be substituted in 2020, which results in zero renewable chemicals production. In the 'Bio + H₂' scenario, the demand grows from zero in 2020 to 250 PJ in 2050. Excess renewable electricity used for producing H₂ and electrochemical ethylene, and wheat for producing succinic acid represent important feedstocks for 2050. The use of syngas from the gasification of biomass residues for producing methanol is competitive in the short and medium terms but as excess electricity increases, methanol is more cost-effectively produced using H₂ derived from the electrolysis of water in the long term. As shown in Figure 3, in 2050, the GHG abatement cost of methanol produced from forest residues is lower than from H₂ using electrolysis of water, but because of system effects (i.e. forest residues are better used in the power and heat sectors for achieving GHG targets), methanol from H₂ derived from electrolysis of water is preferable. For the

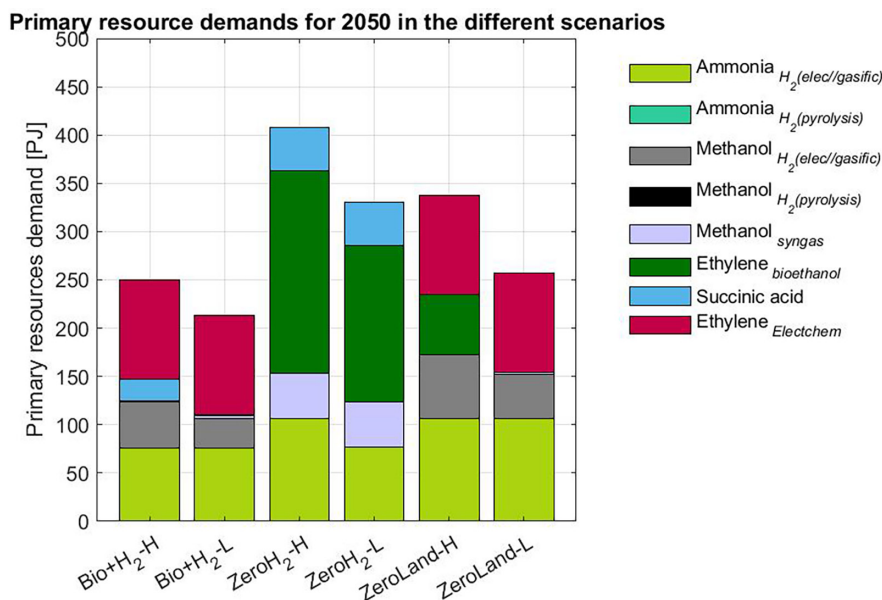


FIGURE 6 Renewable chemicals primary resources demand PJ in the considered scenarios. Bio + H₂ is the scenario in which all primary resources are considered, in ZeroH₂, renewable H₂ from the electrolysis of water and ZeroLand, agricultural land linearly reduces to zero in 2050. L and H represent the lower and higher rate of recycling. Ammonia_{H₂(elec/gasific)} and methanol_(elec/gasific) represent ammonia and methanol produced using renewable H₂ derived from the electrolysis of water or gasification of biomass while ammonia_{H₂(pyrolysis)} and methanol_{H₂(pyrolysis)} represent ammonia and methanol produced using H₂ from biomethane pyrolysis. Methanol_{syngas} is methanol produced using syngas derived from the gasification of biomass. Ethylene_{Electchem} is ethylene produced from the electrochemical reduction of biogenic CO₂.

ZeroH₂ scenario, H₂ for ammonia production is supplied via biomass gasification while for methanol production, syngas from biomass gasification is cost-competitive compared with hydrogen from biomass gasification. In the ‘ZeroLand’ scenario, the total demand for primary resources is 26% higher than in the Bio + H₂ scenario. Generally, the production of H₂ from the pyrolysis of biomethane for the subsequent use in methanol and ammonia production is found not to be cost-effective across all scenarios.

As a result of increased recycling of chemical end products, resulting in recycling of biogenic carbon, the demand for primary resources that would ensure net-zero GHG emissions, decreases by 12%, 20% and 22% for the ‘Bio + H₂’, ‘ZeroH₂’ and ‘ZeroLand’ scenarios, respectively.

3.3 | Sensitivity analysis

The sensitivity of the GHG abatement costs to uncertain input parameters and the influence of input parameters on the GHG abatement costs in 2050 is shown in Figure 7. Bioethylene and succinic acid show the highest variation in terms of abatement costs, which can be explained by the high uncertainty of the input parameter ‘Arable land’ (i.e. 0–1.5Mha). The median abatement

costs for competitive chemicals in 2050 ranges between 500 and 800 €/tCO₂eq. The variability in the rate of recycling of biogenic carbon has the highest impact on the GHG abatement costs, followed by investment costs, excess electricity price, and the biomass feedstock price development. The uncertainty of the remaining parameters shows a small influence on GHG abatement costs in 2050.

4 | DISCUSSION

In this study, the potential role of German biomass potentials and renewable H₂ derived from the electrolysis of water using excess renewable electricity, biomass gasification and biomethane pyrolysis route, towards net-zero GHG emissions by 2050 was investigated. Based on the analysis of the ethylene, ammonia, methanol and adipic acid subsectors, the following key observations are summarized.

4.1 | GHG abatement costs and implications

The practical implementation of a net-zero GHG emissions target for the considered chemicals is challenging

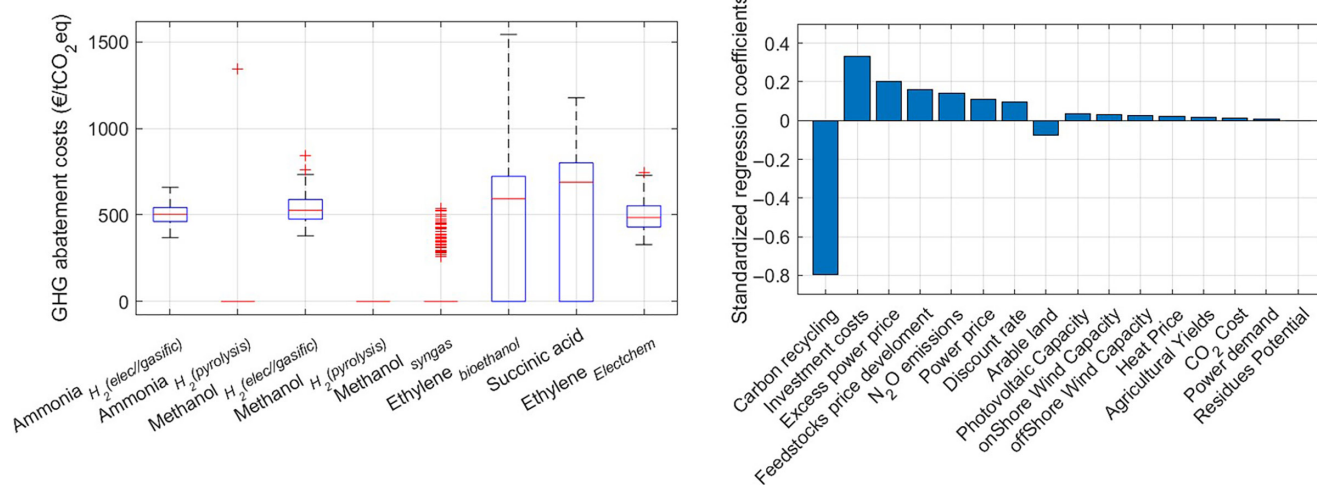


FIGURE 7 Greenhouse gas abatement costs sensitivities to uncertain input parameters from Monte Carlo simulations (left) and the influence of input parameters on greenhouse gas abatement cost (right). Ammonia_{H₂(elec/gasific)} and methanol_{H₂(elec/gasific)} represent ammonia and methanol produced using renewable H₂ derived from the electrolysis of water and biomass gasification. Methanol_{syngas} is methanol produced from syngas produced from biomass gasification. Ethylene_{Electchem} is ethylene produced via the electrochemical reduction of captured biogenic CO₂.

and would probably not materialize without deliberate governmental support. The production costs for the renewable chemicals considered in this work have been found to be 1.3–8 times higher than their fossil counterparts, with feedstock costs contributing the biggest share of the overall costs. Across the considered scenarios, for the year 2050, the marginal GHG abatement cost for the chemicals sector is between 640 and 900 €/tCO₂-eq. The CO₂ prices necessary to make renewable chemicals cost-competitive compared with fossil counterparts in 2050 range between 0 and 810 €/tCO₂-eq. CO₂ prices are expected to vary across different studies due to the different assumptions for the development of fossil primary resources and the feedstocks costs for renewable chemicals, however, the CO₂ costs calculated in this work are similar to those in (Zibunas et al., 2022). This implies that in order to facilitate a net-zero GHG emissions transition, for the considered chemicals (using biomass resources and H₂ produced from excess renewable electricity) by 2050, a marginal CO₂ cost of 480 €/tCO₂-eq levied on fossil counterparts could be enough for their competitiveness. At the time of writing, the CO₂ price in Europe of 90 €/tCO₂ (Bloomberg, 2022; Trading Economics, 2022), would need to increase by more than a factor more than six by 2050.

However, the implementation of such a CO₂ tax on fossil chemicals could risk carbon leakage when similar CO₂ taxes are not imposed in other chemical-producing countries because investors could shift production to areas where it is cheaper to produce. This challenge has been recognized by the EU and a proposal in the ‘Fit for 55’ package regarding a carbon border levy has been

made (Nicholls, 2021). The extent, however, to which this could tackle the problem of carbon leakage should be further investigated because not all chemicals and chemical products are meant for the German market (Workman, 2021).

Unless renewable targets or a cap on fossil fuel usage is in place, such high CO₂-prices might make it attractive to continue using fossil fuels for chemical production, and compensate for emissions through negative emissions achieved elsewhere in the energy system, which may be less costly overall (Millinger, Reichenberg, et al., 2022).

4.2 | The important role of C storage for a net-zero GHG emissions chemicals sector

In scenarios that mimic the limiting of global warming to 1.5°C by 2050, the capture and permanent storage of CO₂, thereby resulting in negative emissions, plays an integral role (IPCC, 2018). This is partly because at the current trajectory, the carbon budget, that is the cumulative global GHG emissions, appears to be likely exceeded and additionally, there are sectors which are difficult to decarbonize such as aviation, whose emissions need to be offset. Technologies that would be able to capture CO₂ and permanently store it, also referred to as negative emissions technologies, would offset emissions in sectors/subsectors where decarbonization is difficult.

For the chemicals industry, which is characterized by diverse product portfolios which do not always have a direct replacement via the renewable route, renewable organic

chemicals could play a decisive role in ensuring net-zero emissions even with hard-to-replace fossil chemicals being produced to some extent. In this work, for the status quo, all the demand for propylene, butadienes, 50% of adipic acid and 40% of ethylene (see Figure 8) could be met by fossil production whilst still achieving net-zero emissions by 2050.

For plastics and polymers, at their end of life, landfilling permanently stores C embedded in them and recycling on the other hand stores C by transferring it to the next value chain.

Considering the current global plastic waste management (OECD, 2022), 50% of renewable C embedded in chemical products could be permanently stored. In the European context, however, where the policy is that, recycling should take precedence over landfilling (European Commission, 2018), deliberate steps to support recycling should be taken. In their work, Stegmann et al. (2022) have shown that a global circular economy with a combined approach of recycling with higher biomass use could ultimately turn the plastics sector into a net carbon sink. In our work, if, for instance, the demand for hard-to-replace chemicals is met by renewable options (assuming an advance in technologies for renewable propylene, butadienes, benzene etc.), this would translate into increased 'carbon sink capacity' which could offset emissions from other sectors such as aviation. However, for this to happen, there has to be a corresponding increased use of biomass combined with carbon

capture through which biogenic CO₂ is made available for methanol and electrochemically produced ethylene. In this work, the available biogenic CO₂ from bioenergy limits the amount of chemicals that can be produced (see Figure 9).

4.2.1 | Carbon recycling

The recycling of C embedded in chemical end products could theoretically be achieved through carbon capture and utilization (CCU), that is when chemical end products are incinerated for energy recovery at their end of life, or through mechanical and chemical recycling processes. Between chemical and mechanical recycling, taking into consideration that renewable C has to be stored and not released as CO₂ in order to guarantee negative emissions, chemical recycling is better suited. Chemical recycling ensures that chemical end products could hypothetically be recycled infinitely while for mechanical recycling, this is only possible 3–7 times (Barrett, 2020). Additionally, chemical recycling has an advantage over mechanical recycling of being able to handle low-quality recyclates (Cefic, 2020). On the other hand, in terms of costs, Volk et al. (2021) report that chemical recycling can be 3 times more expensive compared to mechanical recycling. However, considering that the two recycling routes yield different products, chemical recycling performs better because the net cost (i.e. revenue)

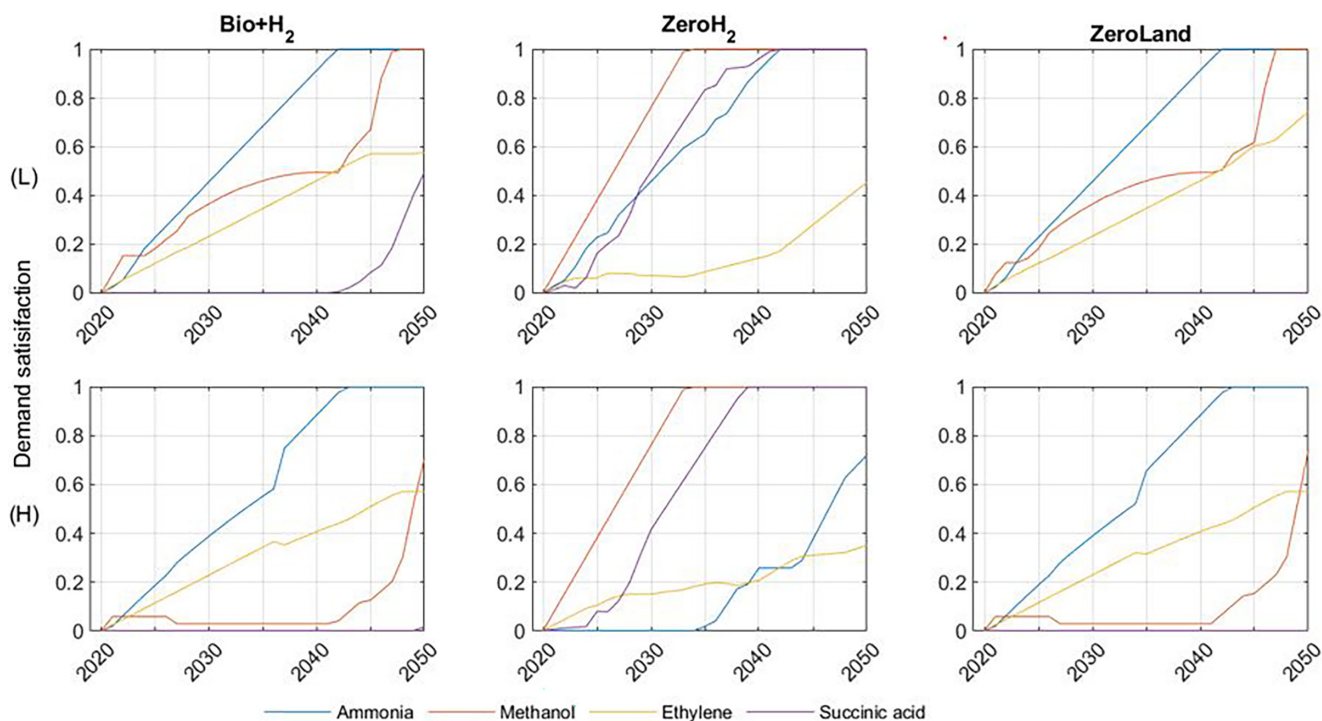


FIGURE 8 Demand satisfaction by the renewable chemicals for the considered chemicals subsectors. Bio + H₂ is the scenario in which all primary resources are considered, in ZeroH₂, renewable H₂ from the electrolysis of water and ZeroLand, agricultural land linearly reduces to zero in 2050.

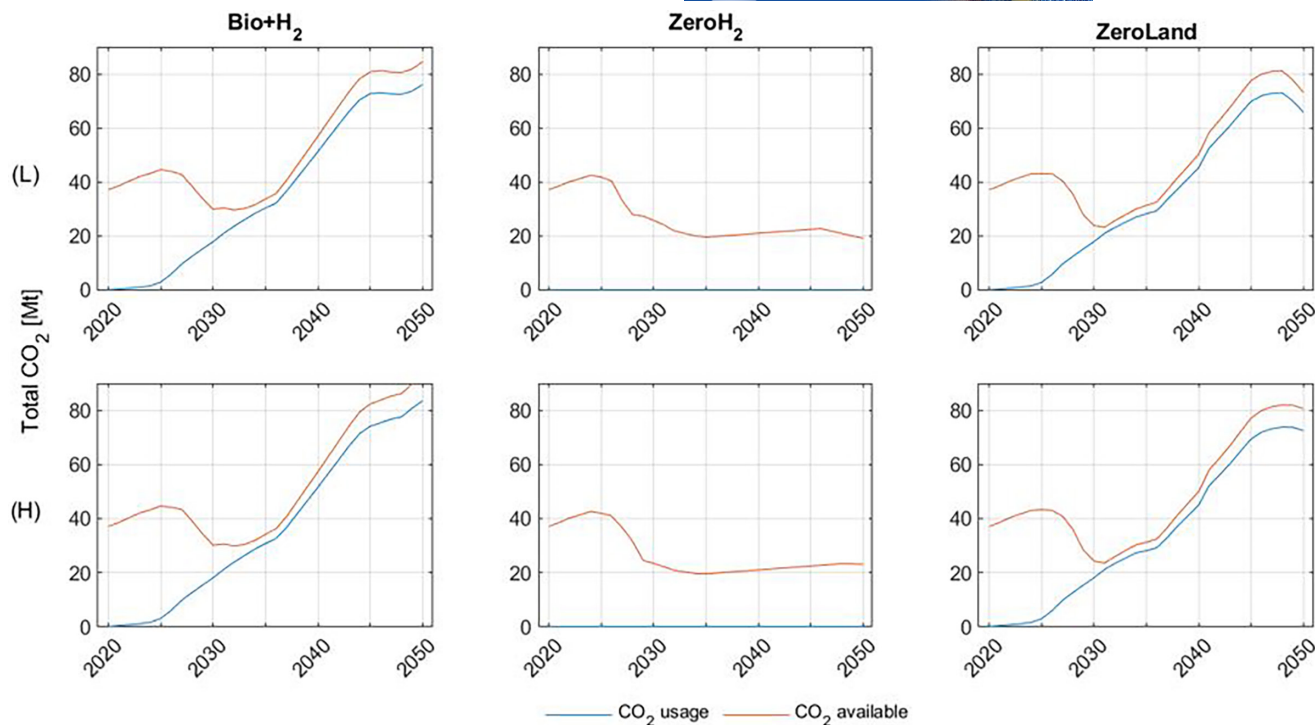


FIGURE 9 Theoretical biogenic CO₂ available from the power and heat sectors and the CO₂ usage by the renewable chemicals. In the figure, Bio + H₂ is the scenario in which all primary resources are considered, in ZeroH₂, renewable H₂ from the electrolysis of water and ZeroLand, agricultural land linearly reduces to zero in 2050.

is $-0.24\text{€}/\text{kg}$ plastic waste compared to $-0.16\text{€}/\text{kg}$ plastic waste for mechanical recycling (Volk et al., 2021).

The costs associated with CO₂ capture vary depending on the CO₂ source, that is whether the CO₂ being produced is concentrated or diluted (Baylin-Stern & Berghout, 2021). For power production which is characterized by dilute CO₂ streams, the costs of CO₂ capture ranges between 40 and 120 $\$/\text{tCO}_2$. With respect to recycling, for a combination of mechanical and chemical recycling in Germany, a cost of $0.14\text{€}/\text{kg}_{\text{input}}$ has been reported by Volk et al. (2021) in a scenario in which the combined recycling potential is enough to reach EU and German recycling targets where plastics are not incinerated for energy recovery.

4.3 | Primary resource demand for net-zero emissions in 2050

For net-zero emissions target for the considered chemicals across the considered scenarios, results indicate that 220–410 PJ of biomass and excess renewable electricity which would classically be available for the energy sectors in 2050, are instead used for the chemicals sector. This would be enough to offset all emissions in basic chemicals production routes except for the Benzene, Toluene and Xylene (i.e. BTX) routes. While achieving targets in the chemicals sector, this cascading use of biomass approach (i.e. maximum material use of biomass) could on the other hand interfere

with overall bioenergy targets by depriving the sector of needed biomass resources (Philp & Winickoff, 2018). Therefore, in order to ensure that bioenergy targets are simultaneously achieved, increased focus could also be placed on maximizing the use of the technical potential for biomass residues, for which 29%–40% of the technical potential remains unused (Brosowski et al., 2016).

The use of biomass resources (i.e. via methane pyrolysis) to produce renewable H₂ which is eventually used to produce ammonia and methanol was not found to be cost-competitive. This is expected considering that this route involves more conversion steps and is thereby more resource and cost-intensive.

4.4 | Comparison with other studies

Although we show that it is possible to achieve net-zero emissions for the considered chemicals, as was also shown by DECHEMA and FutureCamp (2019), there are differences in the approaches that need to be highlighted. Our scope is smaller compared to the scope in (DECHEMA & FutureCamp, 2019) in the sense that they considered all basic chemicals. Additionally, in this work, we incorporate the system effects of the competition for primary resources with the energy sectors. Their results for the fossil GHG emissions and the required abatement are higher than in this work. This is mainly because they considered

the carbon embedded in the chemicals for the total emissions calculation (i.e. 1.37 tCO₂/t of methanol), whilst in our work we assume different levels of recycling of carbon at the end of life of the chemicals end products, which ensures that the carbon is not emitted as CO₂. This, we find to be an important ingredient for reducing the abatement costs for the considered chemicals (i.e. 13%–27%) and we conclude that the recycling industry will be an important partner for a net-zero GHG emissions in 2050. The production of renewable H₂ from electrolysis of water was based on excess renewable electricity in our work whilst in their work, for net-zero GHG emissions, no restriction for electricity available for electrolysis of water was set.

4.5 | Uncertainty analysis

Some input parameter uncertainties could, to a certain degree, be eliminated through certain policy interventions while this is difficult for others. For investment costs, which have been found to have a high influence on the GHG abatement costs in this work, the level of uncertainty could be reduced via increased funding for research and development. Additionally, annualized investment costs can also be reduced through a policy that deliberately reduces the discount rate for renewable chemicals such as reduced interest rates on loans for renewable chemicals infrastructure investments. The discount rate was found to have a significant influence on the GHG abatement cost in this work. The carbon recycling uncertainty could be reduced through a strict recycling mandate on all end products of renewable chemicals. For N₂O emissions, the uncertainty could be reduced by formulating a deliberate policy that could compel farmers to use nitrification inhibitors whenever they use nitrogenous fertilizers. Formulation of such directives should, however, take into consideration the additional costs and how this could translate into the final price of feedstocks.

The uncertainty of other parameters such as biomass feedstock price development, electricity price and excess electricity price which have a strong influence on the cost of GHG abatement, is difficult to reduce through policy or other interventions. This is because values for these parameters are determined by market forces (i.e. supply and demand) and are challenging to influence directly by policy interventions.

4.6 | Research limitations and future directions

Due to the need for model simplification and in order to keep computation time short, the model used in this work

lacks spatial details. Excess electricity generation occurs in specific locations (e.g. more wind in the northern and more solar in the southern parts of Germany), therefore, H₂ production in our model could consider the spatial dimension to improve the assessment. Also, electricity trade between countries could decrease the excess electricity. However, sector coupling studies show that flexible demand such as hydrogen production through electrolysis decreases the need for transmission grid capacities as electricity can be used flexibly near the generation.

5 | CONCLUSION

The aim of this work was to analyze the cost implications of a net-zero GHG emissions for the basic chemicals sector (i.e. ethylene, ammonia, methanol and adipic acid) in Germany and the effect of carbon recycling on GHG abatement costs.

The work concludes that without deliberate governmental support, the practical implementation of a net-zero GHG emissions target for 2050 for the considered chemicals could be challenging. Feedstock costs represent the major cost driver for the total costs, which have been found to be 1.3–8 times higher than the costs of fossil counterparts. For 2050, the costs translate into CO₂ prices ranging between 0 and 480 €/tCO₂-eq which implies that the current CO₂ price in Europe would need to increase by more than a factor of six by 2050. To avoid carbon leakage as a result of such a high CO₂ price, an extension of the carbon border adjustment mechanism, as implemented by the EU for selected imported products, could be an effective supporting measure. If permitted, such high CO₂ prices might incentivize a continued use of fossil fuels for chemicals production, compensated with negative emissions elsewhere in the energy system.

The chemicals sector has a potential to become a net carbon sink which could offset emissions even in hard-to-decarbonize sectors such as aviation, provided that captured biogenic C is available in sufficient amounts to produce chemicals at scale and most importantly, provided that the C embedded in chemical products is permanently stored and not released as CO₂. Waste management policy in the EU discourages landfilling, leaving recycling as a key option for guaranteeing C storage by passing C to the next value chain. Depending on the lifetime of the chemical end products, renewable C could be stored for over 80 years and can further be stored for multiple time periods like this after being recycled. According to this work, the recycling of C resulting in 80% C storage compared to 50% (i.e. global status quo) results in more GHG abatement which further translates into reduced abatement costs of 13%–24% and reduced primary resource demand of 12%–22%.

AUTHOR CONTRIBUTIONS

Frazer Musonda: Conceptualization; methodology; modelling; data curation; writing—original draft; preparation; writing—review & editing; visualization. **Markus Millinger:** Methodology; writing—review & editing; supervision; funding acquisition. **Daniela Thrän:** Resources; writing—review & editing; supervision; funding acquisition.

ACKNOWLEDGEMENTS

This research work was funded by the Federal Ministry of Education and Research, grant number 031B0281A-031B0281II. Open Access funding enabled and organized by Projekt DEAL.

CONFLICT OF INTEREST STATEMENT

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

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available in the supporting information of this paper and at <https://doi.org/10.1016/j.softx.2022.101264> (Millinger, Tafarte, et al., 2022).

ORCID

Frazer Musonda  <https://orcid.org/0000-0001-6184-7078>

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

How to cite this article: Musonda, F., Millinger, M., & Thrän, D. (2024). Modelling assessment of resource competition for renewable basic chemicals and the effect of recycling. *GCB Bioenergy*, 16, e13133. <https://doi.org/10.1111/gcbb.13133>