Cost-optimal pathways towards net-zero chemicals and plastics based on a circular carbon economy

Author(s):
Zibunas, Christian; Meys, Raoul; Kätelhön, Arne; Bardow, André

Publication date:
2022-06

Permanent link:
https://doi.org/https://doi.org/10.3929/ethz-b-000544034

Originally published in:
Computers & Chemical Engineering 162, https://doi.org/10.1016/j.compchemeng.2022.107798

Computers and Chemical Engineering 162 (2022) 107798

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Cost-optimal pathways towards net-zero chemicals and plastics based on a circular carbon economy

Christian Zibunas[a], Raoul Meys[a,b], Arne Kätelhön[a,b], André Bardow[a,c,d,*]

[a] Institute for Technical Thermodynamics, RWTH Aachen University, Aachen 52062, Germany
[b] Carbon Minds GmbH, Cologne 50933, Germany
[c] Institute of Energy and Climate Research - Energy Systems Engineering (IEK-10), Forschungszentrum Jülich GmbH, Jülich, Germany
[d] Energy & Process Systems Engineering, ETH Zurich, Zurich 8092, Switzerland

ARTICLE INFO

Article history:
Received 5 November 2021
Revised 21 February 2022
Accepted 1 April 2022
Available online 9 April 2022

Keywords:
Circular economy
Chemicals and plastics
Transition pathways
Net-zero greenhouse gas emissions
Techno-economic analysis
Carbon pricing
Sustainable Development Scenario

ABSTRACT

Without disruptive change, greenhouse gas (GHG) emissions from fossil production of chemicals and plastics will double by 2050. The transition to net-zero GHG emissions requires a concerted strategy for the whole chemical industry due to its integrated supply chains. A cost analysis is needed to determine the required investments and to design carbon-pricing incentives. Here, we present cost-optimal investment pathways for the global production of chemicals and plastics by using a bottom-up process model that captures the complexity of the chemical industry. To accomplish net-zero, capital expenditures need to increase by 36-51 % over the next 30 years. In contrast, the total annualized cost could be similar (+4 %) to fossil-based production. Net-zero production and its costs will rely on the availability of renewable electricity and biomass. At the same time, high recycling rates are a key to keeping resource demands low and reducing the sensitivity to high resource prices.

1. Introduction

Plastic production consumes over 80 % of all carbon-containing chemicals (Gielen et al., 2008). These chemicals are currently produced from fossil resources accounting for 6 % of global greenhouse gas (GHG) emissions (Ritchie and Roser, 2021). The global demand for plastics is expected to reach 1100 Mt per year in 2050 (World Economic Forum, Ellen MacArthur Foundation and McKinsey and Company, 2016). Thus, remaining fossil-based plastic production would use 15 % of the estimated carbon budget to keep global warming below 1.5 °C by 2050 (World Economic Forum, Ellen MacArthur Foundation and McKinsey and Company, 2016). To stop global warming, the chemical industry must change its production.

The chemical industry can mitigate its GHG emissions by decarbonizing its fossil-based energy supply (Agora Energiewende and Wuppertal Institut, 2019; Geres et al., 2019; International Energy Agency, 2018a) and by deploying low-emission technologies. Low-emission technologies substitute fossil carbon-feedstock using either biomass (European Commission, 2018; Lee et al., 2019; Ögmundarson et al., 2020; Zhang et al., 2020), CO_2 (Carus et al., 2020; d'Amore and Bezzo, 2020; Hepburn et al., 2019; Jens et al., 2019; Kätelhön et al., 2019) or plastic waste (Geyer et al., 2017; Klemeš et al., 2021; Quantis, 2020; Rahimi and García, 2017; Zheng and Suh, 2019). While low-emission technologies already exist at high Technology Readiness Levels, higher investment and operating costs have been reported (International Energy Agency, 2013, 2018a; Material Economics, 2019).

To compensate for the higher costs of low-emission technologies, governments start to price GHG emissions, e.g., via emission trading schemes or carbon tax, encouraging low-carbon investments. For now, most investments seem to focus on the decarbonization of the energy sector (International Energy Agency, 2019; McCollum et al., 2018; Zheng and Suh, 2019). However, the chemical industry will also need substantial investments to start a pathway towards net-zero chemicals and plastics. At the start of this

Abbreviations: BAU, Business-as-Usual Scenario; Bio, biomass; CAPEX, capital expenditures; CCS, carbon capture and storage; CCU, carbon capture and utilization; Elect, electrification; GHG, greenhouse gas; IEA, International Energy Agency; OPEX, operational expenditures; Rec, recycling; SDS, Sustainable Development Scenario; TAC, total annualized costs; TCM, Technology Choice Model; USD, United States Dollar; WACC, weighted average costs of capital.

* Corresponding author at: Energy & Process Systems Engineering, ETH Zurich, Zurich 8092, Switzerland.
E-mail address: abardow@ethz.ch (A. Bardow).

https://doi.org/10.1016/j.compchemeng.2022.107798

pathway, policymakers seek quantification of the necessary investment and carbon pricing to reach net-zero chemicals and plastics (McCollum et al., 2018).

Previous research on the chemical industry assessed environmental impacts and economics for individual GHG mitigation measures (Adnan and Kibria, 2020; Hepburn et al., 2019; Jiang et al., 2020). However, processes of the chemical industry are highly interconnected in existing supply chains. To account for these interconnections, bottom-up models have been used to assess environmental impacts and economics on a regional scale (Agora Energiewende and Wuppertal Institut, 2019; Material Economics, 2019; Schneider and Saurat, 2020). However, previous bottom-up models have not assessed investment decisions of the global chemical industry towards net-zero GHG emissions. Thus, a comprehensive investment pathway for the global chemical industry under carbon pricing is missing.

Here, we calculate transition pathways from 2020′s production levels using fossil technologies towards net-zero GHG emissions by 2050. For this purpose, we develop a techno-economic bottom-up model of the chemical industry. We expand our model (Meys et al., 2021) by operating and investment costs. The model covers the production of 18 large-volume base chemicals and 14 large-volume plastics, accounting for over 75 % of the GHG emissions from global chemical production (International Energy Agency, 2013) and 90 % of the global plastic production volume (Geyer et al., 2017; Zheng and Suh, 2019). Resource and carbon prices are adapted from the International Energy Agency's *Sustainable Development Scenario* (*SDS*) (International Energy Agency, 2018b). Based on the extended model, we minimize the net present costs of the chemical industry between 2020 and 2050 to derive cost-optimal transition pathways. First, we calculate a cost-optimal transition pathway based on the *SDS*'s resource and carbon prices. Then, we study the pathway's sensitivity to varying resource prices. Furthermore, we adjust carbon prices to incentivize pathways to net-zero GHG emissions by 2050 for four combinations of low-emission technologies: (1) A cost-optimal combination of technologies based on electrification (including carbon capture and utilization) and recycling, (2) electrification and biomass, (3) biomass and recycling, and (4) a cost-optimal combination of all technologies. For the four net-zero pathways, we discuss the cumulated capital expenditures from 2020 until 2050, technology choices, corresponding GHG emissions, as well as total annualized costs and resource consumption in 2050.

Our results show that carbon prices between 190 and 370 USD/$t_{CO2\text{-}eq}$ can incentivize the chemical industry to accomplish net-zero GHG emissions by 2050. For this purpose, investments need to increase by 37-51 % compared to a fossil-based *Business-as-Usual Scenario*. In contrast, total annualized costs (TAC) could be similar to fossil-based production under currently forecasted low-end carbon pricing. For a cost-optimal combination of technologies, the chemical industry would build on 62 EJ of biomass, 32 EJ of renewable electricity, and 37 EJ of plastic waste. High recycling rates are a key to reducing resource demands and avoiding strong sensitivity to prices for renewable electricity and biomass.

2. Methods to calculate cost-optimal transition pathways

To derive transition pathways of the chemical industry, we define the chemicals and plastics within the scope (Section 2.2), general assumptions valid for all calculations (Section 2.3), scenarios to cover a broad range of potential pathways (Section 2.4), and the mathematical framework to calculate cost-optimal pathways of the chemical industry towards net-zero GHG emissions (Section 2.5 and 2.6).

2.1. Chemicals and plastics within the scope

Our chemistry industry model covers 18 large-volume base chemicals, 14 large-volume plastics, and the treatment of corresponding plastic wastes (Supplementary Methods 3). In total, the model consists of more than 400 processes based on engineering-level data. Thereby, we consider flows of energy and materials throughout entire supply chains. For a detailed description of included processes, we refer to Meys et al. (2021). In the present study, we expanded the model with operational and capital costs (Supplementary Methods 2 & Supplementary Table 1).

2.2. General assumptions

Main assumptions relate to included GHG emissions (Section 2.3.1), the status quo of the chemical industry in 2020 (Section 2.3.2), investment decisions (Section 2.3.3), and carbon pricing (Section 2.3.4).

2.2.1. Included GHG emissions

GHG emissions are calculated as CO_2-equivalents (CO_2-eq) according to the IPCC GWP 100 (Edenhofer et al., 2014). We include GHG emissions from the production and the end-of-life of chemicals and plastics. For production-related GHG emissions, we include GHG emissions directly from the chemical plants as well as from upstream processes, supplying energy, intermediate products, and raw materials. Footprints of resources, i.e., energy carrier and raw materials, are based on the original bottom-up from (Meys et al., 2021) and stem from Ecoinvent version 3.6 (Ecoinvent, 2020), except for electricity. The electricity footprint depends on the later introduced scenarios. GHG emissions from transport are neglected. To account for GHG emissions occurring during the use phase or the end-of-life, we model the end-of-life as combustion of the chemical's carbon content. Even though low-emission technologies produce identical chemicals, the end-of-life needs to be modeled to account for carbon pricing correctly. For the example of methanol, methanol from fossil fuels is taxed with a carbon price when burned, whereas "renewable" methanol is not taxed, e.g., bio- or CO2-based methanol. This carbon tax at the end-of-life provides a financial incentive to shift to "renewable" methanol. The GHG emissions from the end-of-life are assigned to the chemical's production year. This assumption can be considered conservative regarding annual GHG emissions. A chemical's life cycle could end later and/or the end-of-life might not release the complete carbon content. For plastics, we model GHG emissions of the end-of-life according to literature data (Geyer et al., 2017): Landfilling rates are assumed to decrease from 49 % in 2020 to 6 % in 2050 (Geyer et al., 2017), while recycling and energy recovery rates in 2020 are 23 % and 28 %, respectively. The recycling and energy recovery rates from 2020 until 2050 are determined by cost optimization. Quantities and types of the treated plastic waste are presented in Supplementary Table 3. As we model plastic waste treatment as part of the chemical industry, we include the waste treatment's costs and GHG emissions and potential energy recovery from waste incineration.

2.2.2. Status quo of 2020

For the status quo of the chemical industry in 2020, we include the best available fossil-based technologies, i.e., the industrialized technologies with the lowest costs per kilogram product. Thereby, we underestimate the cost of the fossil-based chemical industry to assess the cost-driven deployment of low-emission technologies conservatively. For all plants existing at the beginning of the transition pathway, we assume a uniform age distribution for plants producing the same chemical. Since the plants will go out of operation once they reach their lifetime, the assumed uniform age

distribution implies that the same production volume will retire for each chemical each year. In line with the literature, existing and new plants are assumed to have a lifetime of 30 years (Seto et al., 2016). Therefore, we assume for each chemical that 1/30 of the production volume already existing in 2020 expire each year. In reality, chemical plants might even exceed the maximum age of 30 years but will need significant refurbishments. Here, we approximate the refurbishment costs to make a plant operatable for another 30 years by the costs of deploying a new plant. The refurbishment costs are due as a single payment when the plant's lifetime expires. Modeling refurbishment in this way is thus identical to the investment in a new plant. Thereby, assuming a strict age limit for plants also includes potential lifetime extension.

2.2.3. Investment decisions

Technologies are chosen to minimize the overall costs of the chemical industry. Thereby, we represent cost-driven investment decisions in the chemical industry. Following the literature on energy systems (E3Modelling, 2018; Loulou et al., 2016), we utilize the net-present-value method to calculate costs, including the capital costs' depreciation, operating costs and costs from carbon pricing. The net-present-value method requires an interest rate, often represented by the weighted average costs of capital (WACC) (E3Modelling, 2018; International Energy Agency, 2020; Loulou et al., 2016). In line with the literature, we assume a WACC of 8% for investments in the chemical industry (Geres et al., 2019; International Energy Agency, 2018b, 2020). To calculate transition pathways towards 2050, we assume perfect foresight on future costs and perfect investor behavior, which is common practice for modeling transition pathways of the energy sector (E3Modelling, 2018; Loulou et al., 2016). Assuming perfect foresight and investor behavior, we assess the potential of optimal investment decisions instead of estimating the outcome of imperfect decisions. However, imperfect decisions may result for the global chemical industry from lack of information, myopic decision-making, or company-specific goals. Regarding company-specific goals, further research could assess the impact of multiple players and objectives within the chemical industry (Avraamidou et al., 2020).

In this study, investments occur in three cases: (1) A plant's lifetime expires, and thus the plant needs to be replaced; (2) A plant is replaced before its lifetime expires because keeping the existing fossil-based technology is more expensive than investing in the corresponding low-emission technology; (3) Growing demand calls for additional plants. For the consumer demand of each chemical, we assume a constant annual growth rate, with values between 1.2 and 5 % for the studied chemicals (ICIS, 2017; Bazzanella and Ausfelder, 2017; International Energy Agency, 2013) (Supplementary Table 2).

Furthermore, the chemical industry's investment volume per year is unlimited. Thereby, we derive the optimal time to substitute fossil-based technologies. With limits, investments will be distributed around the optimal time, and thus the transition will be smoother. However, the sequencing of technology changes will remain the same.

The capital expenditures presented in this work (Fig. 3) represent the capital expenditures needed to build all the plants on the pathway to net-zero GHG emissions and do not consider salvage values of plants that have not expired their lifetime by 2050.

2.2.4. Carbon pricing

In this study, carbon prices refer to the price per emission allowance. We assume that the chemical industry has to purchase allowances corresponding to its annual GHG emissions, including the production and end-of-life of chemicals. Following the literature (Laing et al., 2014), we assume external markets, e.g., the electricity sector, to pass through their costs due to carbon pricing to the chemical industry. Thereby, we incorporate GHG emissions and related costs from upstream processes into the chemical industry's investment decisions.

In contrast to most current emission trading schemes, we include carbon pricing for end-of-life emissions of chemicals. Thereby, we account for emerging carbon taxes, which assign costs to a product according to the product's carbon content. In line with most current emission trading schemes, we exclude biogenic GHG emissions from carbon pricing to account for the carbon uptake during the biomass's growth phase. In the same way, we account for the uptake of CO_2 for carbon capture and utilization (CCU).

2.3. Scenarios for prices, footprints, and available technologies

In this study, we focus on six scenarios: A *Business-as-Usual scenario* (*BAU*), a *Sustainable Development Scenario* (*SDS*), and four scenarios where the chemical industry reaches net-zero GHG emissions by 2050, so-called net-zero pathways. All scenarios are transition pathways based on cost-optimal investment decisions. The scenarios differ with respect to resources prices and footprints, carbon prices, and available technologies.

The *Business-as-Usual scenario* is a reference scenario: The chemical industry remains fossil-based and maintains the current recycling rate of 23 % until 2050, i.e., the cost optimization is constrained to only fossil-based technologies and the recycling rate of 23 %. Resource costs and footprints, and carbon prices correspond to the *Sustainable Development Scenario (SDS)* described next.

The *Sustainable Development Scenario* represents a potential pathway of the chemical industry under carbon pricing. In this scenario, the chemical industry can combine all fossil and low-emission technologies on a cost-optimal basis. Resource prices and carbon pricing are based on the eponymous scenario of the International Energy Agency (International Energy Agency, 2018b). The IEA's scenario includes prices for crude oil, natural gas, and electricity (Supplementary Table 4) but does not include biomass prices. Thus, we derive biomass prices from the literature. In this study, we model biomass as energy crops represented by miscanthus. Corresponding biomass prices cluster around $<$100–200 USD/t_{dry} (Alonso et al., 2017; Geres et al., 2019; Lewandowski et al., 2018; Sanchez et al., 2015a) with outliners of 50 and 279 USD/t_{dry} (International Energy Agency, 2020; Khanna et al., 2008). We assume a constant biomass price of 200 USD/t_{dry} to conservatively assess the deployment of bio-based technologies in a cost-driven industry. In reality, the biomass price would vary over time and by region, for example due to difference in demand and supply. If a high demand is paired with a scarce supply, price elasticity will increase the biomass price. Our model does not reflect a price elasticity. However, the biomass price assumed in this study is already at the top-end of the literature data and, therefore, might represent the prices under high demand.

Resource footprints are based on (Meys et al., 2021), except for electricity. The electricity footprint is adopted from the IEA's scenario (Supplementary Table 4), which considers grid-electricity.

For the four net-zero pathways, we change the electricity's footprint and costs, available technologies, and carbon prices. Previous literature already emphasized that electrification can only be economically (Hepburn et al., 2019) and environmentally (Meys et al., 2021) competitive when using low-cost renewable electricity. The grid electricity from the *Sustainable Development Scenario* might not achieve sufficient low costs and footprints. In contrast, off-grid electricity might accomplish desirable costs and footprints. Thus, in the net-zero pathways, we assume that the chemical industry will have access to renewable off-grid electricity from wind and solar power by 2030 (Supplementary Table 4). In this study, assuming access to off-grid electricity refers to a chemical industry

that only consumes electricity at low price (36 USD/MWh) and low carbon footprint (20 g_{CO2eq}/kWh). This assumption could represent either of the following three designs of the chemical industry: A chemical industry, where (1) production sites are directly linked to a solar field or wind park, (2) the electricity-demanding process steps, e.g., hydrogen electrolysis, are outsourced to regions, with high solar and/or wind intensity, (3) or the decarbonization of the grid electricity achieves corresponding low price and emission parameters. Our model does not reflect the effect of such setups on plant design and operation. Thus, our model reflects a best-case with low-price, low-emission electricity.

For each of the four pathways, we include a different combination of available technologies to assess the influence of technology and resource availability: A cost-optimal combination of technologies based on (1) electrification, including carbon capture and utilization, and recycling (*Elect + Rec*), (2) electrification and biomass (*Elect + Bio*), (3) biomass and recycling (*Bio + Rec*), and (4) a combination of biomass, electrification, and recycling (*All*).

Technologies based on biomass include fermentation to ethanol with subsequent conversion to ethylene, gasification to synthesis gas (2:1), and combustion for steam generation. Technologies based on electrification include electrical steam generation and heating, water electrolysis to hydrogen, and CCU-processes for methane and methanol with the option for subsequent conversion to olefins or aromatics. For CO_2 sources, we modeled the highly-concentrated point sources from the conventional ammonia production, steam methane reforming, and ethylene oxide production as well as from biomass fermentation and gasification. At the same time, direct air capture is used to conservatively approximate all further potential CO_2 sources (e.g., from utilities).

Pathways labeled with recycling allow recycling rates higher than in the *Business-as-Usual Scenario*. Recycling technologies include mechanical recycling of packaging waste, and chemical recycling to monomers or naphtha. Furthermore, all net-zero pathways allow conventional fossil technologies and waste treatment via landfilling or energy recovery. The technology choice of all pathways is subject to cost-minimization (Section 2.3.3). Supplementary Table 1 includes a detailed list of all technologies.

The technologies are combined based on the following reasoning: The pathway combing all circular technologies, by definition, shows the overall cost-optimal transition pathway to net-zero. However, the pathway will only provide insight into the most cost-competitive technologies. Thus, we want to assess further subsets of all low-emission technologies. For this purpose, we clustered the available low-emission technologies by their dominant energy sources, which are biomass, electricity, and plastic waste. Pathways based on single energy sources would be an obvious choice to give further insight. However, single energy sources, on their own, fail to enable net-zero GHG emissions. Therefore, we assessed each possible combination of two energy sources. Thereby, the absence of one of the three energy sources can be assessed to give further insights.

Carbon capture and storage (CCS) was excluded from all scenarios to focus on circular carbon technologies. However, we discuss the potential role of CCS in Section 3.4. We adjust carbon prices for each combination of low-emission technologies to incentivize a cost-optimal deployment of the available low-emission technologies so that the chemical industry accomplishes net-zero GHG emissions by 2050.

2.4. Computational structure of the static bottom-up model

To derive net-zero pathways, we expand the Technology Choice Model (TCM) (Kätelhön et al., 2016) to model the transition of the chemical industry's production over time. Thus, we first describe the structure of the original static TCM and, after that, its expansion.

The TCM follows the general notation of Life Cycle Assessment (Heijungs and Suh, 2002), and describes the production system by five basic entities: (1) technologies, (2) intermediate flows, (3) the final demand, (4) elementary flows, and (5) monetary flows. Technologies are defined as processes transforming inputs into outputs. Intermediate flows include all flows between technologies, such as raw materials, energy, intermediate products, and products for final consumption. The amounts of products for final consumption are specified as the final demand. Elementary flows include all flows between technologies and the environment, such as GHG emissions or resources extraction. Monetary flows include all expenses to operate plants, i.e., the capital costs' depreciation, operating costs, and carbon pricing costs.

We structure the data on the production system according to the generalized calculus for Life Cycle Assessment (Heijungs and Suh, 2002). The technology matrix A describes the transformation of intermediate flows by technologies. In this matrix A, columns represent production technologies, while rows represent intermediate flows. A coefficient a_{ij} of the technology matrix A indicates the production (for $a_{ij} > 0$) or consumption (for $a_{ij} < 0$) of the intermediate flow i by the technology j. Analogously, the elementary flow matrix B describes the exchange of elementary flows between technologies and the environment. In this matrix B, a coefficient b_{ej} describes the emission (for $b_{ej} > 0$) or extraction (for $b_{ej} < 0$) of an elementary flow e by technology j. Likewise, the costs to operate technologies are described by the cost matrix F. In this matrix F, a coefficient f_{mj} describes the monetary flow m that was spent ($f_{mj} > 0$) or earned ($f_{mj} < 0$) due to the operation of the technology j. The final demand vector y, describes the final demand for intermediate flow i.

The production system has to meet the final demand. Therefore, the scaling vector s scales each technology's inputs and outputs and determines the production level to meet the final demand. To choose the most cost-efficient technologies, we introduce a linear optimization problem:

$$\min\ Z = \sum_{m=1}^{n} Fs \tag{1}$$

$$s.t.\ As = y \tag{2}$$

$$s \geq 0 \tag{3}$$

$$s \leq c \tag{4}$$

The objective function Z is minimizing the sum of all costs of the chemical industry, Eq. (1). The constraints ensure producing the final demand, Eq. (2). All entries in s must be positive. Otherwise, a process could convert products into inputs, Eq. (3). Furthermore, we include upper bounds, Eq. (4), to incorporate treatment scenarios for plastic waste and restrict the deployment of low-emission, e.g., low-emisson-technologies are restricted in the scenario *BAU*.

Based on the optimal solution for the scaling vector s, we can calculate the GHG emissions of the cost-optimal chemical industry:

$$g = Bs \tag{5}$$

$$h = QBs \tag{6}$$

The vector s scales the exchange of elementary with the environment per process, Eq. (5). The characterization vector Q, characterizes the exchange of elementary flows regarding their contribution to climate change, Eq. (6). Thus, in Q, an element q_e represents the 100-year global warming potential of elementary flow e, according to the IPCC methodology (Edenhofer et al., 2014).

2.5. Dynamic expansion of the technology choice model

The static TCM optimizes the chemical industry for one time step only and thus cannot be used to derive a transition pathway. Therefore, we expand the TCM to optimize multiple future time steps based on cost-optimal investment decisions. For this purpose, we incorporate the net-present-value method in three steps: (1) We introduce variables for investment decisions to a single time step; (2) we replicate the equations of the single time step to model all time steps of the transition pathway, (3) we introduce constraints that model dependencies between all time steps, i.e., plants can only operate if they were built in the past and have not already been decommissioned.

The resulting optimization to derive cost-optimal investment pathways is structurally similar to the static optimization problem:

$$\min Z = \sum_{m=1}^{n} (F^{**} . * d^{**}) s^{**} \tag{7}$$

$$s.t.\ A^{**} s^{**} = y^{**} \tag{8}$$

$$C^{**} s^{**} \leq b^{**} \tag{9}$$

$$s^{**} \geq 0 \tag{10}$$

$$s^{**} \leq c^{**} \tag{11}$$

The Eqs. (8), (10), and (11) are structurally the same as in the static optimization problem, with matrices and vectors expanded for investment decisions and for multiple timesteps (indicated by the double asterisk). Furthermore, we add a discount vector d^{**} to the objective function to incorporate the net-present-value method. Eq. (9) represents that plants can only operate if they were built in the past and have not already been decommissioned. Details on the expansion of the matrices and the resulting model are presented in Supplementary Methods 1.

3. Results and discussion

Section 3.1 introduces the fossil reference scenario and discusses the influence of resource and carbon prices on cost-optimal transition pathways. In Section 3.2, we assess capital expenditures of transition pathways to net-zero GHG emissions. Section 3.3 explores technology choices of net-zero pathways. Then, we discuss residual emissions (Section 3.4), total annualized costs (Section 3.5), and resource consumption (Section 3.6) of net-zero supply chains in 2050. Finally, we discuss the availability of renewable resources (Section 3.7) and the influence of recycling on the chemical industry (Section 3.8).

3.1. Sustainable development scenario and carbon pricing incentivizes for net-zero GHG emissions

In the *Business-as-Usual Scenario* (*BAU*), the chemical industry remains fossil-based and maintains the current recycling rate of 23 % until 2050. Consumer demands for chemicals are expected to increase until mid-century (on average +3.1 %/a) (Supplementary Table 2). If the production of chemicals remains fossil-based, growing demands will increase the global chemical industry's annual GHG emissions from 2.1 $Gt_{CO2\text{-}eq}$ in 2020 to 5.5 $Gt_{CO2\text{-}eq}$ in 2050, cumulating to a total of 106 $Gt_{CO2\text{-}eq}$ between 2020 and 2050 (Fig. 1).

To meet climate goals suggested by the Intergovernmental Panel on Climate Change, the chemical industry needs to turn net-zero by 2050. However, cost-optimal investment decisions currently favor fossil-based production over a net-zero supply chain due to lower total annualized costs. Thus, the chemical industry will need incentives to transition to net-zero, e.g., carbon pricing.

The International Energy Agency's (IEA) *Sustainable Development Scenario* (*SDS*) suggests a linear increase in carbon pricing from 25 USD/$t_{CO2\text{-}eq}$ in 2020 to 190 USD/$t_{CO2\text{-}eq}$ in 2050. The IEA's calculations forecast all sectors to mitigate 70 % of 2018 global CO_2 emissions by 2050. Thereby, the global industry would be on track to net-zero by 2070 (International Energy Agency, 2018b). According to our calculations with the carbon and resource prices adapted from the IEA's *SDS*, annual GHG emissions of the chemical industry decrease by 63 % from 2020 to 2050 (Fig. 1, red line). The decrease is similar to the IEA's projections, where all sectors mitigate 70 % of 2018′s GHG emissions. Thus, carbon prices increasing to 190 USD/$t_{CO2\text{-}eq}$ do not incentivize a net-zero chemical industry by 2050.

However, the influence of carbon prices on investment decisions and corresponding GHG emissions depends on the assumed resource prices. A sensitivity analysis on resource prices shows the range of the chemicals industry's transition pathways under the *SDS*'s carbon prices (Fig. 1, grey area). Under upper-end cost for oil (143 USD/barrel) and natural gas (8.2 USD/GJ) combined with low-end costs for biomass (100 USD/t_{dry}) and electricity (26 USD/MWh), reaching net-zero GHG emissions would be cost-optimal by 2029. In contrast, the chemical industry would reduce its annual GHG emissions of 2050 by only 17 % compared to the *Business-as-Usual Scenario* when assuming low-end cost for oil (50 USD/barrel) and natural gas (4.9 USD/GJ) combined with upper-end costs for biomass (279 USD/t) and electricity (79 USD/MWh) (Supplementary Methods 4).

To incentivize a transition to net-zero by 2050, carbon pricing can be adjusted to each set of resource prices. If resource prices strongly favor fossil production, carbon pricing needs to be more ambitious. In contrast, less favorable fossil resource prices can be paired with lower carbon prices and still incentivize net-zero GHG emissions by 2050, Fig. 2. Furthermore, the necessary carbon prices depend on the availability of technologies and resources. Therefore, we analyze the required carbon prices for four combinations of technologies (Fig. 2): A cost-optimal combination of (1) electrification (including CCU) and maximal recycling (*Elect + Rec*), (2) electrification and biomass (*Elect + Bio*), (3) biomass and maximal recycling (*Bio + Rec*), and (4) a cost-optimal combination of all circular technologies (*All*). Combinations without maximal recycling still maintain the recycling rate of the *Business-as-Usual Scenario* at 23 %. Since carbon prices are adjusted to incentivize net-zero by 2050, carbon price trajectories differ between the net-zero pathways. Thus, earlier GHG mitigation (in Fig. 1) should not be interpreted as a pathway outperforming another but higher carbon prices making the low-carbon technologies cost-competitive earlier.

Under the resource prices of the IEA's *SDS*, necessary carbon prices range from 199 up to 817 USD/$t_{CO2\text{-}eq}$ depending on the employed technologies. The lowest carbon price at 199 USD/$t_{CO2\text{-}eq}$ suffices when combining all three technology categories (All) or biomass with high recycling rates (Bio + Rec). The necessary carbon prices are equal since the cost-optimal combination of all technologies does not include any electrification-based technologies when assuming the *SDS*'s resource prices. Electricity prices are too high to compete with biomass and recycling.

Comparing the combination of all technologies (*All*) with electrification and biomass (*Elect + Bio*) shows the impact of recycling. High recycling rates reduce necessary carbon pricing from 323 to 199 USD/$t_{CO2\text{-}eq}$.

The combination of electrification and recycling (*Elect + Rec*) needs the highest carbon prices at 817 USD/$t_{CO2\text{-}eq}$. The high

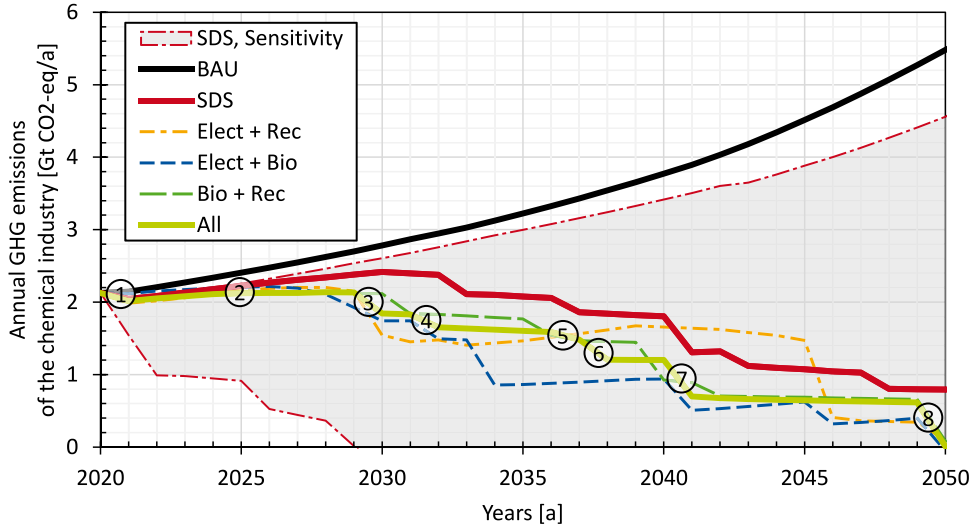

Fig. 1. Annual GHG emissions for potential transition pathways of the chemical industry until 2050. The *Business-as-Usual Scenario* (*BAU*) represents a fossil-based reference where the recycling rate from 2020 (23 %) remains constant until 2050. The *Sustainable Development Scenario* (*SDS*) is a cost-optimal transition pathway based on resource and carbon prices from the eponymous scenario of the International Energy Agency. The grey area shows the sensitivity of cost-optimal pathways to resource prices when keeping the *SDS*'s carbon prices. Four additional pathways show cost-optimal transition pathways for four different combinations of technologies, where carbon prices are adjusted to incentivize net-zero GHG emission by 2050: A combination of (1) electrification, including carbon capture and utilization, and recycling (*Elect + Rec*), (2) electrification and biomass (*Elect + Bio*), (3) biomass and recycling (*Bio + Rec*), and (4) a combination of biomass, electrification, and recycling (*All*). Numbers indicate the replacement of remaining depreciated fossil-based plants with low-emission technology for the pathway combining all technologies (*All*): 1 mechanical recycling, 2 chemical recycling via pyrolysis, 3 bio-based methanol, 4 electrical steam generation, 5 shutdown of waste incineration, 6 hydrogen from electrolysis for ammonia production, and resistance heaters, 7 bio-based ethylene, 8 propylene from bio-based ethylene (For references to colors in this figure, please see the web version of this article.).

	Oil	NG	Biomass	Electricity	Elect + Rec	Elect + Bio	Bio + Rec	All
	[$/barrel]	[$/GJ]	[$/t]	[$/MWh]	Necessary carbon prices [USD/$t_{CO2\text{-}eq}$/a]			
high renewable vs. low fossil	50	3.9	279	**79**	912	513	375	375
SDS	**70**	**5.5**	**200**	**79**	817	323	199	199
SDS with off-grid electricity	**70**	**5.5**	**200**	36	370	304	199	190
low renewable vs. high fossil	140	7.1	100	26	266	52	57	21

Fig. 2. Necessary carbon prices in 2050 to incentivize net-zero GHG emissions by 2050. Carbon prices are adjusted to incentivize a transition to net-zero GHG emissions by 2050 when assuming costs-optimal investment decisions. The necessary carbon prices depend on the assumed resource prices and the available technologies. Resource price scenarios include the IEA's *Sustainable Development Scenario* (*SDS*), an adaptation of the *SDS*, where electricity is approximated by cheap off-grid electricity, and two extreme scenarios, where upper-end fossil prices are compared to low-end renewable prices and vice versa. Prices in this figure depict the 2050′s prices. For all prices between 2020 and 2050 see the Supplementary Table 4. For each scenario of resource prices, we assess four combinations of technologies: A cost-optimal combination of technologies based on (1) electrification, including carbon capture and utilization, and recycling (*Elect + Rec*), (2) electrification and biomass (*Elect + Bio*), (3) biomass and recycling (*Bio + Rec*), and (4) a combination of biomass, electrification, and recycling (*All*). Bold numbers indicate the original resource prices of the IEA's SDS. NG = Natural Gas, Oil = Crude Oil.

prices mainly result from the electricity price of the IEA's *SDS*. In the *SDS,* the electricity is assumed to be grid-electricity at 79 USD/MWh. Previous research already emphasizes the low economically (Hepburn et al., 2019) and environmental (Meys et al., 2021) competitiveness of electrification when using grid electricity. Thus, we also introduce a scenario *SDS with off-grid electricity*, where the chemical industry has access to off-grid electricity at 36 USD/MWh by 2030. All other prices of the original *SDS* remain unchanged.

Due to the lower electricity prices, necessary carbon prices decrease by 55 % for the combination of electrification and recycling (*Elect + Rec*). The influence on the other combinations is smaller as the electricity consumption is lower. Despite the introduction of cheaper off-grid electricity, the ranking of combinations by their carbon prices remains unchanged, indicating a lower cost-competitiveness of complete electrification. However, electrification-based technologies are now part of the optimal combination of all technologies (*All*) since they become cost-competitive at 36 USD/MWh electricity prices.

Besides electricity, changes in other resource prices influence the necessary carbon prices as well. The extrema of carbon prices result when comparing upper-end fossil resource prices with low-end renewable resource prices and vice versa. Necessary carbon prices can be as low as 21 or as high as 912 USD/$t_{CO2\text{-}eq}$.

In summary, necessary carbon prices strongly depend on resource prices and the combination of low-emission technologies. Consequently, regional differences in the availability and prices of resources will determine the most desirable low-emission technologies and the corresponding needs for carbon pricing incentives. However, regional differences in carbon pricing also bear the risk of carbon leakage. Carbon leakage has to be contained to incentivize net-zero chemical production worldwide, e.g., via carbon-border adjustments. Otherwise, fossil-based production may shift to regions with mild carbon pricing and continue emitting greenhouse gasses.

Suppose carbon leakage is contained and the chemical industry has access to biomass at 200 USD/$t_{CO2\text{-}eq}$ and electricity at 36 USD/MWh. In that case, carbon prices of 190-370 USD/$t_{CO2\text{-}eq}$ can incentivize net-zero GHG emissions by 2050. These carbon prices are in the predicted range for certificate prices of the emission trading scheme in the European Union and mid-century social carbon cost (European Commission, 2011; Ricke et al., 2018). Social

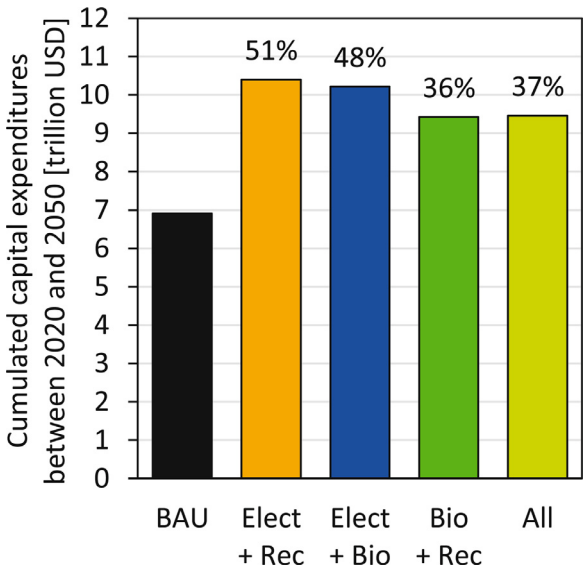

Fig. 3. Cumulated capital expenditures of the global chemical industry between 2020 and 2050. In the *Business-as-Usual Scenario* (*BAU*), the chemical industry invests in replacing decommissioned plants and building new production capacities to satisfy growing consumer demands. The other scenarios show the capital expenditures of the chemical industry to reach net-zero emissions by 2050 for four combinations of available technologies based on (1) electrification, including carbon capture and utilization, and recycling (*Elect + Rec*), (2) electrification and biomass (*Elect + Bio*), (3) biomass and recycling (*Bio + Rec*), and (4) biomass, electrification, and recycling (*All*).

carbon costs depict society's costs due to climate change impacts. Being in the range of social carbon costs indicates that a transition to net-zero chemicals would be socio-economically appealing even without carbon pricing.

In the following sections, we assess pathways to net-zero GHG emissions in more detail. We focus on the net-zero pathways based on the *Sustainable Development Scenario with off-grid electricity* since previous research already emphasized the low competitiveness of electrification when using grid electricity, like in the *SDS* (Hepburn et al., 2019; Meys et al., 2021).

3.2. Capital expenditures to accomplish a transition to net-zero GHG emissions

In the *Business-as-Usual Scenario*, the chemical industry spends 6.9 trillion USD between 2020 and 2050 to replace decommissioned plants and satisfy growing consumer demands. The calculated investment is similar to extrapolations from past investments (6.1 trillion USD) (Supplementary Table 5) (Cefic, 2020). Investments for research and innovation might add another 1.4 trillion USD (Cefic, 2020) to the required investment but are not included in Fig. 3. The chemical industry uses 34 % of the total 6.9 trillion USD to replace decommissioned plants. The chemical industry uses the remaining 66 % building new plants to satisfy growing consumer demands (on average +3.1 %/a).

To accomplish net-zero GHG emissions, the chemical industry has to invest 9.4–10.4 trillion USD over the next 30 years, corresponding to 2.5–3.5 trillion USD (36–51 %) more capital than in the *Business-as-Usual Scenario* (Fig. 3). Combining electrification and recycling is the most capital-intense pathway (+51 %) as electrification is the most capital-intense GHG mitigation strategy. In contrast, the combination of biomass and recycling is the least capital-intense strategy at +36 %. When combining all strategies, the chemical industry's investments are even 1% higher (+37 %), while operating costs are reduced to accomplish the overall lowest total costs over the invested period. All in all, the range of capital-intensity for net-zero chemicals increase the capital intensity similar to the energy sector's decarbonization (15–50 %) (Gielen et al., 2019; International Energy Agency, 2018b; International Energy Agency and International Renewable Energy Agency, 2017).

Necessary capital might come from governments, banks, and households, as awareness of climate change and commitment to climate goals increases (McCollum et al., 2018). For instance, BlackRock, a multinational investment management corporation, has pledged to direct more investments to climate-friendly enterprises (BlackRock, 2021). BlackRock currently manages over 9 trillion USD in assets and thereby, on its own, already exceeds the additional capital needs of the chemical industry (CNBC, 2021). In 2020, BlackRock's customers invested 288 billion USD in sustainability-oriented financial products, more than doubling the additional investment need of net-zero chemicals (83-117 billion USD/a) (BlackRock, 2021). Also, governments plan to acquire capital for mitigating climate impacts, e.g., the EU plans to mobilize 0.9 trillion USD over the next decade (European Commission, 2020). On an annual basis, the EU's investment would be 90 billion USD, which is in the range of the additional investment needs of the chemical industry. The chemical industry most certainly will not be the only sector looking for low-carbon investments. However, being in the same range as planned investments of single players suggests that capital acquisition could be a feasible task.

3.3. Technologies deployment of net-zero pathways

The four net-zero pathways (Fig. 1) are derived assuming cost-optimal investment decisions. Investment decisions are based on the resource prices of *the Sustainable Development Scenario with off-grid electricity*, and the carbon prices are matched to incentivize net-zero for each combination of technologies (Fig. 2). By definition, the pathway combing all circular technologies shows the overall cost-optimal transition to net-zero. A mix of all three GHG mitigation strategies is optimal: recycling, biomass usage, and electrification. In the following, we focus on this pathway for analyzing the timing of investment decisions and technology choices. However, for each technology choice, we discuss possible alternatives from the other pathways.

The transition pathway shows disruptive changes in GHG emissions (marked by numbers in Fig. 1). Disruptive changes result when a low-emission technology substitutes all corresponding depreciated fossil plants. This substitution only occurs if the low-emission technology's total annualized costs are lower than the operational costs of the already depreciated fossil plant. Before each disruptive change, the operational costs of the low-emission technology and the fossil technology break even. After the break-even point, the chemical industry gradually deploys the low-emission technology to replace decommissioned fossil plants or satisfy growing demands. This gradual deployment lowers the GHG emissions' gradient compared to the *Business-as-Usual Scenario* in Fig. 1. During such gradual deployment, GHG emissions can still increase since consumer demands continuously grow. Only recycling cannot replace all fossil plants during a disruptive change since the amount of treatable waste is insufficient to substitute all virgin production. Each year virgin plastic production exceeds the amount of waste due to growing consumer demands, the long life cycle of non-packaging plastics, and losses during the life cycle (Geyer et al., 2017).

The disruptive changes occurring in *the Sustainable Development Scenario with off-grid electricity* using all technologies are discussed in the following based on the numbering introduced in Fig. 1:

(1) In 2021, the chemical industry deploys additional mechanical recycling plants and recycles 169 Mt of packaging waste returning from the use phase (polyethylene, polypropylene, polystyrene, and polyethylene terephthalate). This amount corresponds to all

the global packaging waste included in this study (Supplementary Table 3). Thereby, the cost-optimal pathway suggests deploying mechanical recycling as much as possible. In reality, the deployment might be slower, on which we expand in more detail in Section 3.9. By introducing more mechanical recycling, the chemical industry replaces fossil polymer production and mitigates GHG emissions. Until 2050, the mitigation potential of mechanical recycling will grow with the increasing amount of packaging waste returning from the use phase (Supplementary Table 3). The remaining non-packaging waste and residues from sorting and recycling predominantly go to waste incineration and landfills.

Landfilling would have been the cost-optimal choice over recycling and waste incineration with energy recovery due to its lower costs and lower direct GHG emissions in the short term. However, landfilling causes external costs due to long-term GHG emissions (Finnveden and Nielsen, 1999), leakage of heavy metals, and leakage to the marine environment (Borrelle et al., 2020; Lau et al., 2020). Thus, landfilling is regarded as not acceptable. Therefore, landfilling rates are assumed to decrease linearly from 49% in 2020 to 6% in 2050, which is in line with the literature (Geyer et al., 2017).

(2) From 2023 on, at a carbon price of 41 USD/$t_{CO2\text{-}eq}$, the chemical industry gradually deploys chemical recycling via pyrolysis. At first, the chemical industry recycles residues from sorting and mechanical recycling, which previously have been incinerated. From 2027 on, at a carbon price of 63 USD/$t_{CO2\text{-}eq}$, the chemical industry recycles a part of the non-packaging waste. Another part still goes to energy recovery to supply heat and electricity. The deployment of chemical recycling is not disruptive as landfilling rates are assumed to decrease gradually. However, more rapid deployment of chemical recycling would be cost-efficient. By 2050, all pyrolysis processes produce 319 Mt of naphtha per year. The naphtha fuels conventional steam crackers to produce benzene, toluene, and xylene. Without waste pyrolysis, the chemical industry would lack a cheap route to produce benzene, toluene, and xylene, as observed for the pathway *Bio + Elect*. In this case, the chemical industry would need to produce additional methanol for subsequent methanol-to-aromatics conversion.

(3) In 2030, at a carbon price of 80 USD/$t_{CO2\text{-}eq}$, constructing bio-based gasifiers becomes cheaper than running depreciated fossil-based synthesis gas production. In 2050, the chemical industry gasifies 470 Mt_{dry}/a of biomass to synthesis gas for subsequent methanol production. The alternative process to bio-based methanol is CO_2-based methanol production. In the pathway without biomass (*Elect + Rec*), the chemical industry substitutes all fossil-based methanol with methanol from CO_2 and hydrogen from electrolysis at a carbon price of 140 USD/$t_{CO2\text{-}eq}$. Assuming an electricity price of 30 instead of 36 USD/MWh will make CO_2-based methanol the most cost-efficient technology by 2050, while bio-based methanol would act as a bridging technology (Supplementary Fig. 1).

(4) In 2032, at a carbon price of 91 USD/$t_{CO2\text{-}eq}$, electrical steam boilers become cost-competitive compared to methane-based steam boilers. In 2050, the chemical industry will utilize an additional 8 EJ of electricity. The counterpart is bio-based steam production. In the pathway without electrification (*Bio + Rec*), bio-based steam-boilers are fully deployed at 118 USD/$t_{CO2\text{-}eq}$.

(5) In 2037, at a carbon price of 118 USD/$t_{CO2\text{-}eq}$, incentives are sufficient to shut down the remaining waste incineration of non-packaging plastic waste. All non-packaging waste is recycled via pyrolysis, while some residuals from sorting and mechanical recycling still go to waste incineration. In contrast, waste incineration is the dominant waste treatment with 71 % for the pathway without recycling (*Bio + Elect*).

(6) In 2038, at a carbon price of 124 USD/$t_{CO2\text{-}eq}$, the chemical industry replaces decommissioned plants for steam-methane-based ammonia with ammonia synthesis via hydrogen from electrolysis. In 2050, hydrogen electrolysis for ammonia production will consume 11 EJ additional electricity. The bio-based alternative to producing hydrogen would be biomass gasification with a subsequent water gas shift, fully deployed at 153 USD/$t_{CO2\text{-}eq}$ in the pathway without electrification (*Bio + Rec*).

At a carbon price of 124 USD/$t_{CO2\text{-}eq}$ and an electricity price of 36 USD/MWh., it is also cost-competitive to substitute natural gas-based process heat with electricity-based resistance heaters. Resistance heaters have higher abatement costs than electricity-based steam production due to assumed retrofitting costs.

(7) In 2041, at a carbon price of 140 USD/$t_{CO2\text{-}eq}$, substituting all remaining fossil-based ethylene with ethylene from bio-ethanol becomes cost-competitive. A low-carbon alternative would be CO_2-based methanol for subsequent ethylene and propylene production using methanol-to-olefines technology. In a pathway without biomass (*Elect + Rec*), methanol-to-olefins substitutes depreciated fossil ethylene production at a carbon price of 324 USD/$t_{CO2\text{-}eq}$.

(8) In 2050, at a carbon price of 180 USD/$t_{CO2\text{-}eq}$, the chemical industry substitutes all depreciated fossil-based propylene production with propylene from bio-based ethylene. The chemical industry will ferment 3.5 Gt_{dry}/a of biomass for ethanol production with subsequent dehydration to ethylene in 2050. 44 % of the ethylene is designated for propylene production.

In summary, market-ready technologies can enable a pathway to net-zero annual GHG emissions: Mechanical and chemical (pyrolysis) recycling, bio-based ethanol and methanol, the subsequent production of ethylene, propylene, as well as electrical steam production, and the production of ammonia via hydrogen from electrolysis. High-temperature electrical heating via resistance heaters may be the only technology, which is currently not market-ready but is expected to be market-ready by 2035 (Geres et al., 2019). However, since all other technologies are already commercially available, research and technological development will probably not limit the pathway. On the contrary, further development could even improve efficiencies, costs, and remaining emissions. Such improvements could accelerate the transition towards net-zero chemicals based on circular technologies (Geres et al., 2019).

An alternative for a cheap and fast transition to a net-zero GHG emission system could be carbon capture and storage (CCS). The costs of CCS range from less than 20 (Global CCS Institute, 2021) up to 600 USD/$t_{CO2\text{-}eq}$ (Lebling et al., 2021). The lower-end costs can be achieved for highly concentrated CO_2-sources. For example, CCS could be combined with fossil-based ammonia and ethylene oxide, reducing GHG emissions at low costs. Another scenario would be carbon capture at the high-concentration point sources from gasification and fermentation of biomass. The combination with bio-based production could even result in net-negative GHG emissions, similar to bioenergy and carbon storage. In contrast, utilizing dilute CO_2-sources, e.g., CO_2 captured from the air, leads to upper-end costs of 600 USD/$t_{CO2\text{-}eq}$, which are expected to decrease to 200 USD/$t_{CO2\text{-}eq}$ in the future (Lebling et al., 2021). However, CCS is not a circular approach; fossil resources and storage capacities are ultimately limited (Fasihi et al., 2019) (Supplementary Discussion 1). Thus, in the following, we focus on circular technologies only.

3.4. Residual GHG emissions of a net-zero chemical industry

Even though the sum of annual GHG emissions can reach net-zero by 2050, the production of chemicals and plastics would still emit greenhouse gasses. Direct CO_2 emissions from production are offset by the carbon uptake of biomass and CCU technologies. For biomass, this assumption only holds if as much biomass grows back as utilized (Wiloso et al., 2016) and no GHG emissions occur from land-use change. This study assumes biomass from lig-

nocellulosic energy crops cultivated on marginal lands, which regrow fast and are not connected to land-use-change emissions (Lewandowski et al., 2018). However, resource availability will be important for the envisioned large-scale deployment and is therefore discussed in Section 3.7. The carbon uptake can also not offset the residual GHG emissions from biomass cultivation, electricity generation, and non-carbon process emissions, e.g., dinitrogen oxide from biomass gasification.

Despite these residual GHG emissions, two mechanisms enable net-zero annual GHG emissions: (1) Due to an unavoidable landfilling rate of 6 % (Geyer et al., 2017), carbon is stored in landfilled plastics. According to Althaus et al. (2007), we assume plastic waste on landfills only emits 1 % of its carbon content over the next 100 years. Thereby, landfills store 99 % of the carbon content, corresponding to 0.19 $Gt_{CO2\text{-}eq}$/a. However, the carbon content could be emitted later. Thus, landfilling should not be mistaken as permanent carbon storage (Gabrielli et al., 2020). (2) Each year, more plastics enter the stock of in-use plastics than return for their waste treatment (Geyer et al., 2017). Thereby, also the plastic stock acts as a carbon storage corresponding to 0.65 $Gt_{CO2\text{-}eq}$/a in 2050. However, this mechanism will vanish when plastic production reaches a steady-state, where plastic waste equals production volume. However, a steady-state will also lead to a better match of the produced plastics and the availability of plastic waste for recycling. Increasing recycling will lower resource consumption and thus corresponding residual emissions. To ultimately accomplish net-zero without either of the two mechanisms, the chemical industry would need to mitigate residual emissions completely or deploy net-negative technologies, e.g., direct air capture and carbon storage.

3.5. Total annualized costs of net-zero supply chains in 2050

Assuming the resource prices of the *Sustainable Development Scenario with off-grid electricity* (Fig. 2), the total annualized cost (TAC) might increase for net-zero supply chains compared to fossil production (*BAU*). However, the increase in TAC is smaller than the increase of capital expenditures: TAC of net-zero supply chains increase by only 4-18 % compared to fossil production, including currently-forecasted low-end carbon pricing (42 USD/ $t_{CO2\text{-}eq}$, Supplementary Methods 4) (International Energy Agency, 2018b). The highest TAC occur when combining electrification and recycling (18 %), while the lowest costs (4 %) are found for the combination of all circular technologies (*All*). Under the most ambitious carbon pricing from the *Sustainable Development Scenario* (190 USD/$t_{CO2\text{-}eq}$) the TAC of fossil production would increase to 3.8 trillion USD (*BAU*). Then, net-zero supply chains would all outperform the fossil supply chain. Thus, the fossil-based production costs depend strongly on carbon pricing. The potential risk of increased cost through carbon pricing might shift investors from fossil-based production to net-zero products despite the TAC increase by 4 % in the studied base case.

However, all cost contributions are uncertain. The depreciation, fixed operational expenditure, and resource costs contribute 22-27 %, 34-40 %, and 34-40 % to the overall TAC. Depreciation represents the capital intensity of each supply chain. Thereby, improvements for capital expenditures of each deployed technology could change the TAC. Moreover, the depreciation depends on the weighted average cost of capital (WACC), which is assumed to be 8 % in this study. The WACC are known to differ by region and technology (E3Modelling, 2018), e.g., due to varying risk premiums. Fixed OPEX include maintenance, operating supplies, insurances, etc., which also can be subject to uncertainty. The uncertainty of fixed OPEX and the depreciation depend on all technologies of the supply chains and is therefore complex to resolve.

In contrast, the uncertainty of resource costs is defined by the prices of only five resources, so that price changes for a single resource could significantly change the overall cost. Therefore, we study the impact of changes in resource prices on costs. Resources prices may vary due to regional demand and availability. Thereby, the uncertainty bars also represent the possible regional-specific difference. The lower- and upper-end of resource prices are defined by the extrema from Fig. 2. Biomass prices may also differ due to the type of biomass, e.g., energy crops or forest residues. Thus, the uncertainty bars could also represent different biomass types.

Among the net-zero supply chains, the combination of electrification and recycling has the highest uncertainty (Fig. 4). The high uncertainty results from the upper-end electricity prices representing grid electricity. This finding highlights the economic importance of cheap electricity for an electrification-based chemical industry. Combining recycling with biomass instead of electricity results in a smaller uncertainty even though the upper-end biomass prices are represented by outliners from the literature (International Energy Agency, 2020). Combining biomass and electrification as well reduces the price uncertainty compared to electricity and recycling. Moreover, resource reliance is spread over two markets. The inclusion of high recycling rates can reduce uncertainty even further as resource consumption decreases. Thereby, the uncertainty is also smaller for the combined circular technologies compared to the fossil supply chain.

At the lower-end of fossil and renewable resources prices, two net-zero supply chains can break even with the fossil supply chain's TAC of 2.7 trillion USD (even for low-end carbon pricing at 42 USD/$t_{CO2\text{-}eq}$): (1) The combination of all technologies and (2) the combination of biomass and recycling. Biomass and recycling being part of both supply chains indicates their significance for the cost-efficient production of net-zero chemicals. Recycling is particularly important to reduce costs in scenarios with high prices for electricity and biomass.

3.6. Resource consumption of net-zero supply chains in 2050

Low-emission technologies allow reducing the GHG emissions but are usually associated with high resource demands. We, therefore, compare resource demands of net-zero production to fossil-based production (Fig. 5). In 2050, the fossil supply chain (*BAU*) will build on crude oil (71 EJ), natural gas (29 EJ), electricity (2 EJ), and plastic waste (37 EJ). Plastic waste primarily fuels energy recovery plants (23 EJ).

The supply chain based on electrification and recycling builds on electricity (127 EJ) and plastic waste (37 EJ). Compared to the fossil supply chain (*BAU*), resource consumption increases by 18 % measured in terms of exergy content. In contrast, the combination of biomass and recycling consumes 133 EJ, 5 % less than the fossil supply chain. The resource consumption also indicates a higher resource efficiency of bio-based production compared to electrification. When combining all circular technologies, the chemical industry could build on 1 EJ of crude oil, 33 EJ of electricity, 62 EJ of biomass, and 37 EJ of recycled plastic waste. This chemical industry would balance its resource consumption so that neither biomass nor electricity makes more than 50 % of the resource consumption. Furthermore, high recycling rates reduce the overall resource consumption from 160 EJ (*Bio + Elect*) to 134 EJ (*All*): Biomass consumption decreases from 101 EJ to 62 EJ, while electricity consumption slightly increases from 23 EJ to 33 EJ to compensate for the energy recovery. While biomass dominates the resource consumption, a further shift to electrification is possible. Reducing the electricity price from 36 USD/MWh to 26 USD/MWh makes CO_2-based methanol with hydrogen from electrolysis cheaper than bio-based methanol (assuming a fixed biomass price at 200 USD/t_{dry}).

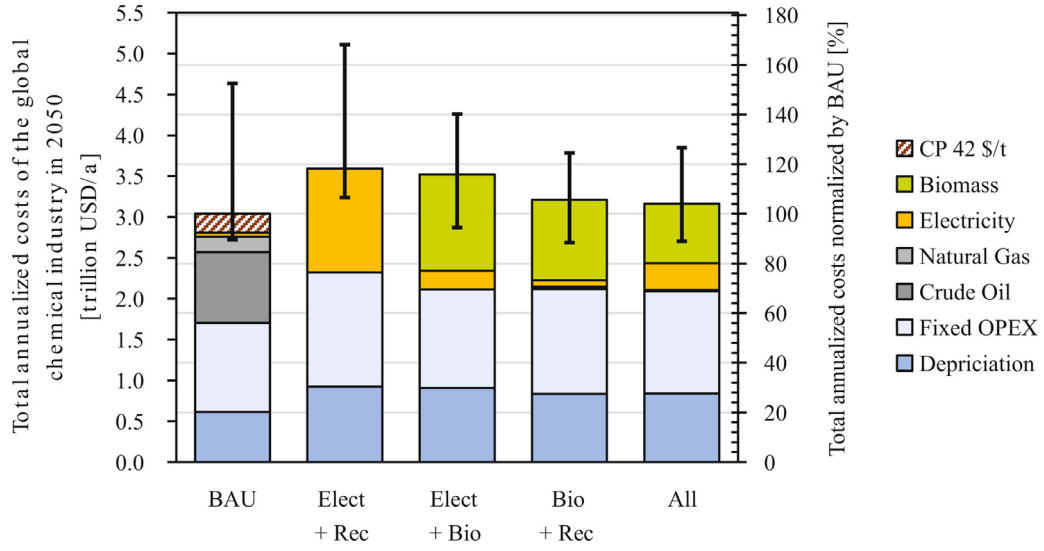

Fig. 4. Total annualized costs of the global chemical industry in 2050. Total annualized costs (TAC) include the depreciation of capital expenditures, fixed operational expenditures (OPEX), costs of resources, and costs due to carbon pricing (CP). Uncertainty bars represent the sensitivity of the TAC to a range of resource prices (Fig. 2). The figure shows costs for low-end carbon pricing (42 $/t$_{CO2\text{-}eq}$, Supplementary Methods 4), while higher costs are possible (Fig. 2). Costs due to carbon pricing only occur for the fossil-based scenario BAU. All other supply chains accomplish net-zero GHG emissions and thus avoid carbon pricing costs. The right axis shows the TAC relative to the scenario *BAU*.

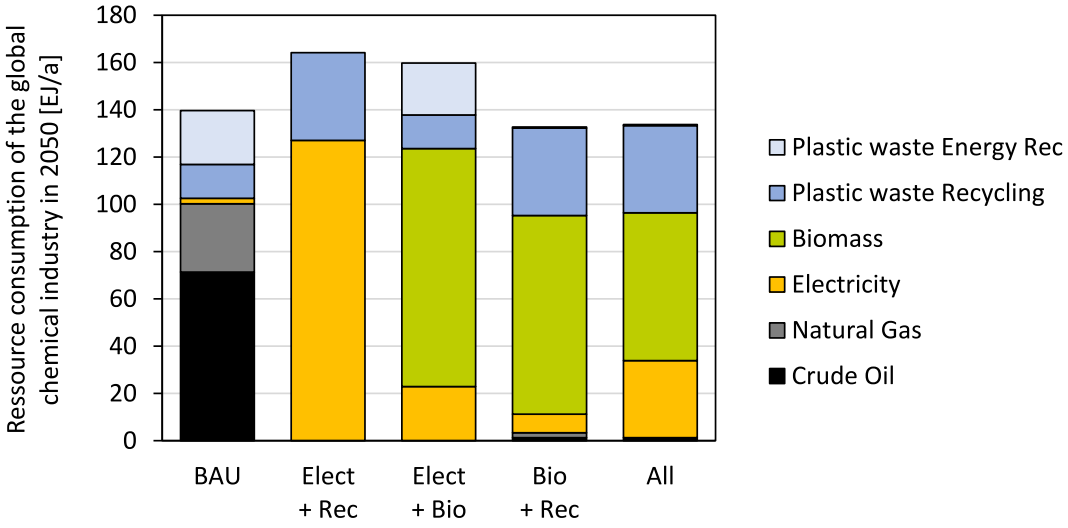

Fig. 5. Resource consumption of the chemical industry in 2050. The chemical industry's resource consumption in 2050, including feedstocks and energy, is compared by exergy content. The BAU represents a fossil-based reference, while the four other bars show the resource consumption of supply chains, which result in net-zero GHG emissions: A cost-optimal combination of technologies based on (1) electrification, including carbon capture and utilization, and recycling (Elect + Rec), (2) electrification and biomass (Elect + Bio), (3) biomass and recycling (Bio + Rec), and (4) a combination of biomass, electrification, and recycling (All).

Thereby, resource demands could shift from 62 to 33 EJ of biomass and electricity to 50 and 49 EJ (Supplementary Discussion 2). Either way, the chemical industry will need access to low-cost and low-emission biomass and electricity. Their availability is therefore discussed next.

3.7. Availability of cheap and sustainable resources

The previous analysis shows the importance of low-cost and low-emission biomass and electricity for transitioning to a net-zero chemical industry. Biomass could significantly influence the GHG emissions and operational costs of net-zero chemicals and plastics. In the literature, biomass prices cluster around 100-200 USD/t_{dry} (Alonso et al., 2017; Geres et al., 2019; Kühner, 2013; Lewandowski et al., 2018; Sanchez et al., 2015a) with outliners of 50 and 279 USD/t_{dry} (International Energy Agency, 2020; Khanna et al., 2008). Even at a biomass price at the upper end of the cost range (200 USD/t_{dry}), total annualized costs of net-zero chemicals are in the range of current fossil-based production (Fig. 4). Thus, cost-competitive biomass processes are likely. To affirm this cost-competitiveness, future research needs to quantify biomass's price elasticity due to the very large biomass demand induced by the chemical industry. If the global demand exceeds the supply, the price elasticity could increase biomass prices. In particular, the chemical industry could be not the only sector relying on biomass for GHG mitigation. However, the biomass price assumed in this study is already at the top-end of the literature data and thus, might as well represent the prices under high demand.

Besides competitive biomass prices, sufficient availability for biomass with a low carbon footprint is essential to realize the promised GHG reductions (Carus et al., 2020). A closed carbon cycle requires that as much biomass needs to regrow as harvested (Wiloso et al., 2016). Otherwise, a carbon debt would be created. In particular, forest wood harvesting will create a carbon debt as regrowing takes several decades (Raven et al., 2021). First-generation biomass promises a faster regrowth but is edi-

ble, and thus, the chemical industry would compete with the food sector.

Using energy crops, such as *Miscanthus* assumed here, allows fast regrowth and does not directly compete for biomass with the food industry (Lewandowski et al., 2018). However, the chemical industry would compete for land to grow biomass. To avoid competition for land, energy crops should only grow on marginal land, not designated for food production (International Energy Agency, 2017). Energy crops could even create economic revenue as the land otherwise might have no economic value (International Energy Agency, 2017). Furthermore, increasing yields of food crops might create surplus land to grow energy crops (Hoogwijk et al., 2003; International Energy Agency Bioenergy, 2007). Estimates of biomass availability from marginal and surplus lands range widely between 0 EJ and ~1000 EJ in 2050 (Hoogwijk et al., 2003; International Energy Agency, 2017, 2020). However, many sources consider 200 EJ of biomass reasonable for sustainable biomass harvesting (International Energy Agency, 2020). As the chemical consumes 62 EJ of biomass for the cost-optimal combination of all circular technologies, it would claim 31 % of the sustainable biomass. Thereby, the chemical industry would not compete with land for food products and leave another 138 EJ of energy crops for other sectors.

For the available biomass, the chemical industry needs to avoid GHG emissions from direct and indirect land-use change, which could compromise bio-based GHG mitigation (International Energy Agency, 2017). Initial literature estimated GHG emissions from land-use change (e.g., deforestation of carbon-rich tropical forests) to completely offset the biomass's carbon uptake (Searchinger et al., 2008). Although subsequent studies have estimated lower GHG emissions from land-use change (Broch et al., 2013), avoiding land-use change is crucial to the success of bio-based GHG mitigation (Harper et al., 2018). If the biomass grows on marginal land, no land elsewhere has to be repurposed, and thus, no indirect land-use change occurs. Still, careful deployment strategies need to be developed to allow for large-scale deployment of biomass. Regarding direct land-use change, energy crops might increase the soil organic carbon content. Thus, net emissions from direct land-use change might be negative (Agostini et al., 2015; International Council on Clean Transportation, 2018; McCalmont et al., 2017). However, potential negative direct land-use change emissions are neglected in this study to conservatively assess the energy crops' carbon footprint. Even though previous research indicates a potentially low price, low footprint, and sufficient availability, energy crops have to prove their economic and sustainable potential on a regional level (Escobar and Laibach, 2021).

Besides biomass, the footprint and costs of electricity generation impact the potential net-zero chemical industry. For the cost-optimal combination of all circular technologies, electricity consumption amounts to 33 EJ. The IEA's scenario estimates electricity generation to increase by 108 EJ for net-zero GHG emissions of all sectors (International Energy Agency, 2020). So, the chemical industry would claim 31 % of the additional renewable electricity. Although the chemical industry's demand lies within the IEA's estimates, it will compete with demands from multiple other sectors, e.g., for e-mobility or hydrogen-based steel production. Thus, acquiring sufficient renewable electricity might be challenging.

Costs and footprints of electricity generation can be especially low for wind and solar power (Agora Verkehrswende, Agora Energiewende and Frontier Economics, 2018). To minimize electricity footprints, full-load hours have to be maximized. Thus, in the future, chemical production might need to move to wind and solar-intense regions if not already located there, e.g., Scandinavia or North Africa. Alternatively, the chemical industry could import electricity or electricity-intensive precursor, like hydrogen and CO_2-based methanol, from those regions. Footprints can further decrease if GHG emissions from the production of solar panels and wind turbines decrease as well, e.g., due to GHG mitigation in copper and steel production.

In summary, resource acquisition will undoubtedly be challenging. However, the estimated demands seem to lie within the range currently deemed feasible. Regional differences in availability and footprints of biomass and electricity will determine operational costs and overall GHG emissions. Careful monitoring could help to select the best resources, which live up to the promise of low footprints for electricity and avoid land-use-change and carbon depts for biomass.

3.8. The role of recycling for a transition towards net-zero GHG emissions

As already emphasized, recycling is a key technology to reduce resource demands and costs. In the following, we compare the net-zero supply chain combining biomass electricity and maximal recycling (*All*) with the supply chain combining biomass and electrification (*Bio + Elect*), where the recycling rate is limited to the 2020′s status quo (23 %). High recycling rates reduce the TAC of the net-zero chemical industry by 10 %. Moreover, biomass consumption decreases by 38 %, and thus net-zero production would rely less on biomass. The lower demand also reduced the sensitivity to biomass prices. Ultimately, a lower resource consumption might facilitate the acquisition of cheap and sustainable resources.

However, recycling has to be promoted globally to accomplish these desirable cost reductions and reduce the cost's sensitivity to high resource prices. So far, global recycling capacities do not match the rapid deployment in recycling plants suggested by the cost-optimal transition pathways. Thus, GHG mitigation would be slower than in the suggested pathways. Therefore, persistent efforts and a continuous increase in recycling capacities seem critical for the chemical industry.

Currently, most plastic waste is either landfilled (50 %) or combusted for energy recovery (27%) (Geyer et al., 2017). Landfill bans have already emerged to increase recycling rates and tackle environmental concerns regarded with landfilling (PlasticsEurope, 2018). Thereby, the availability of plastic waste can also increase. Currently, available plastic waste is mainly used for energy recovery due to lower costs. So far, carbon pricing policies exclude greenhouse gasses from plastics' end-of-life, i.e., from energy recovery. Thus, energy recovery would remain a cheap source of electricity and heat even under high carbon prices. To incentivize GHG mitigation over the whole lifecycle, carbon pricing needs to include GHG emissions from energy recovery of plastic waste. This inclusion would be similar to already existing carbon taxes of fuels. Fuels are taxed by their carbon content, thus accounting for GHG emissions from combustion.

In summary, mitigating landfilling and incorporating end-of-life emissions into carbon pricing could be crucial pillars to support recycling. Where recycling is desirable, further research might help to improve the design and operation of local waste management systems (Mohammadi et al., 2019).

4. Conclusion

This study shows that carbon pricing between 190 and 370 USD/$t_{CO2\text{-}eq}$ in 2050) in combination with biomass at 200 USD/t_{dry} and renewable electricity at 36 USD/MWh can incentivize a cost-optimal transition to net-zero chemicals and plastics by 2050. To accomplish this transition, the chemical industry has to spend 36-51 % more capital compared to fossil-based production. The recent boom of sustainability-supporting investment funds indicates that low-carbon investments are already appealing to investors.

To make investments economically even more appealing, policies could create a predictable and transparent investment environment (Gielen et al., 2019) with low economic risk. For example, subsidized insurances on sustainability investments could mobilize vast amounts of private capital (Schmidt, 2014).

Besides new production plants, investments will be needed for research to improve technology (e.g., reduced energy consumption or increased yields) and new infrastructure (e.g., networks for biomass, electricity, hydrogen, or CO_2). However, infrastructure might be beyond individual companies' scope and thus calls for governmental support (Bruyn et al., 2020). Beyond R&D investments within the chemical industry, technology improvements from other sectors could help the chemical industry (e.g., improved electrolyzer or gasifier from the energy sector).

In contrast to the large additional investments (36-51 %), total annualized costs (TAC) are expected to increase by only 4–18 % compared to the fossil-based production under currently-forecasted low-end carbon pricing. Depending on resource prices, the total annualized cost could also break even or be lower than fossil-based production. Under ambitious carbon pricing, TAC of fossil-based production could even face an increase of 27 % compared to currently forcasted low-end carbon pricing. The potential risk of a 27 % cost increase could discourage investors, while emission-free products might be appealing, even if production costs increase slightly.

For competitive prices and low emissions, policies need to promote sufficient resource availability to exploit the full GHG mitigation potential and counteract high prices due to price elasticity. Simultaneously, policies need to address issues that compromise GHG mitigation, e.g., carbon debts (Wiloso et al., 2016). Addressing sustainability issues in advance should also be accompanied by monitoring the sustainability once renewable resources are used (Gilbert and Sovacool, 2015; Sanchez et al., 2015b).

For biomass, forecasts on availability range widely, and competition for biomass with the energy sector could emerge (International Energy Agency, 2017, 2020). Competition with the energy sector could be reduced by using biomass over multiple product life cycles in the chemical industry before being delegated to energetic use (Stegmann et al., 2020). Regarding biomass footprints, policies should promote crops with fast regrow rates to prevent a carbon debt (Wiloso et al., 2016) and biomass cultivation on marginal lands to prevent land-use change (Escobar and Britz, 2021). Besides GHG emission, policies have to check further sustainability aspects (International Council on Clean Transportation, 2018), such as soil degradation, water use, and biodiversity (Pawelzik et al., 2013).

For renewable electricity, hydrogen from electrolysis with off-grid electricity could provide a cheap and sustainable building block for renewable ammonia production and CCU technologies (Carus et al., 2020; International Energy Agency, 2018a; Kätelhön et al., 2019; Material Economics, 2019). To assure low footprints and high availability, companies could import precursors (e.g., hydrogen or methanol) from wind- and solar-intense regions as they often import fossil feedstock today.

Since renewable electricity and biomass could be scarce, synergies between CCU- and bio-based technologies might help the chemical industry reach net-zero (Bachmann et al., 2021; Meys et al., 2021). Combining electricity and biomass also distributes resource demands onto two resources, while realizing high recycling rates can drive down the overall resource consumption. Recycling can be a crucial pillar to accomplish net-zero chemicals and plastics. Recycling not only drives down resource consumption but thereby also reduces the sensitivity to resource prices. To unleash the potential of recycling, policies could introduce further landfilling bans. Furthermore, carbon pricing needs to include GHG emissions from waste incineration to level the playing field among waste treatment options, which may grant recycling an overall cost advantage in the future. In addition to recycling, policies should also consider reuse of plastics, as so far it is often granted less focus (Klemeš et al., 2021). Strengthened reuse could decrease consumer demands for new plastic and corresponding GHG emissions.

All net-zero pathways still emit greenhouse gasses in 2050, which are offset by storing carbon in the stock of in-use plastics mitigating 0.65 $Gt_{CO2\text{-}eq}$. Thereby, the chemical industry reaches net-zero for annual GHG, but not necessarily over the whole product life cycle. While reaching net-zero of either kind might be desirable, politics have to address the differences to adjust policies and carbon accounting. However, if the chemical industry wants to reach net-zero over the whole product life cycle, all residual GHG emissions, which cannot be mitigated or captured, have to ultimately be offset by net-negative technologies (e.g., direct air capture and carbon storage (Creutzig et al., 2019)).

In this study, we derived multiple cost-optimal investment pathways towards net-zero chemicals and plastics. In summary, the economics of net-zero chemicals appear to be quite promising: Indeed, the capital intensity of net-zero chemicals increases significantly (36–51 %) but so does recent capital acquisition for low-emission investments. TAC could even be similar to current fossil-based production, and necessary carbon pricing incentives might not exceed social carbon costs. The biggest challenge for net-zero might be the availability of renewable resources. However, high recycling rates can reduce overall resource demands and thus could be an essential steppingstone enabling net-zero GHG emission chemicals and plastics.

Declaration of Competing Interest

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

CRediT authorship contribution statement

Christian Zibunas: Writing – original draft, Conceptualization, Methodology, Software, Investigation, Visualization, Data curation, Project administration. **Raoul Meys:** Writing – review & editing, Conceptualization, Methodology, Data curation. **Arne Kätelhön:** Writing – review & editing, Conceptualization, Methodology. **André Bardow:** Conceptualization, Writing – review & editing, Supervision, Resources, Funding acquisition.

Acknowledgments

This work was supported by the Ministry of Economics, Innovation, Digitalization, and Energy of North-Rhine Westphalia [grant number: EFO 0001 G]. The support is gratefully acknowledged.

Furthermore, we thank Benedikt Winter and Patricia Mayer (at Energy & Process Systems Engineering, ETH Zürich) and Marvin Bachmann and Leonard Müller (at Institute for Technical Thermodynamics, RWTH Aachen University) for proofreading and their helpful feedback on this paper.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2022.107798.

References

Adnan, M.A., Kibria, M.G., 2020. Comparative techno-economic and life-cycle assessment of power-to-methanol synthesis pathways. Appl. Energy 278, 115614. doi:10.1016/j.apenergy.2020.115614.

Agora Energiewende, Wuppertal Institut, 2019. Klimaneutrale Industrie: Schlüsseltechnologien und Politikoptionen für Stahl, Chemie und Zement. Agora Energiewende, Wuppertal Institut.
Agora Verkehrswende, Agora Energiewende and Frontier Economics, 2018. The Future Cost of Electricity-Based Synthetic Fuels. Agora Verkehrswende, Agora Energiewende and Frontier Economics.
Agostini, F., Gregory, A.S., Richter, G.M., 2015. Carbon sequestration by perennial energy crops: is the jury still out? Bioenergy Res. 8, 1057–1080. doi:10.1007/s12155-014-9571-0.
Alonso, D.M., Hakim, S.H., Zhou, S., Won, W., Hosseinaei, O., Tao, J., et al., 2017. Increasing the revenue from lignocellulosic biomass: maximizing feedstock utilization. Sci. Adv. 3 (5), e1603301. doi:10.1126/sciadv.1603301.
Avraamidou, S., Baratsas, S.G., Tian, Y., Pistikopoulos, E.N., 2020. Circular economy - a challenge and an opportunity for process systems engineering. Comput. Chem. Eng. 133 (7), 106629. doi:10.1016/j.compchemeng.2019.106629.
Bachmann, M., Kätelhön, A., Winter, B., Meys, R., Müller, L.J., Bardow, A., 2021. Renewable carbon feedstock for polymers: environmental benefits from synergistic use of biomass and CO_2. Faraday Discuss. 230 (9), 227–246. doi:10.1039/D0FD00134A.
Bazzanella, A., Ausfelder, F., 2017. Low Carbon Energy and Feedstock for the European Chemical Industry. DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e.V.
BlackRock. Client Letter, 2021. Net zero: a fiduciary approach 2021. BlackRock.
Borrelle, S.B., Ringma, J., Law, K.L., Monnahan, C.C., Lebreton, L., McGivern, A., et al., 2020. Predicted growth in plastic waste exceeds efforts to mitigate plastic pollution. Science 369 (6510), 1515–1518. doi:10.1126/science.aba3656, New York, N.Y..
Broch, A., Hoekman, S.K., Unnasch, S., 2013. A review of variability in indirect land use change assessment and modeling in biofuel policy. Environ. Sci. Policy 29, 147–157. doi:10.1016/j.envsci.2013.02.002.
Bruyn, S.D., Jongsmam, C., Kampman, B., Görlach, B., Thie, J.E., 2020. Energy-intensive Industries - Challenges and Opportunities in Energy transition. Study For the Committee On Industry, Research and Energy (ITRE), Policy Department For Economic, Scientific and Quality of Life Policies. European Parliament, Luxembourg, p. 2020.
Carus, M., Dammer, L., Raschka, A., Skoczinski, P., 2020. Renewable carbon: key to a sustainable and future-oriented chemical and plastic industry: definition, strategy, measures and potential. Greenh. Gas Sci. Technol. 10 (3), 488–505. doi:10.1002/ghg.1992.
Cefic, 2020. Facts & Figures of the European chemical industry 2020. Cefic.
CNBC, 2021. BlackRock Quarterly Profit Jumps As Assets Rise Over $9 Trillion. CNBC.
Creutzig, F., Breyer, C., Hilaire, J., Minx, J., Peters, G.P., 2019. Socolow R. The mutual dependence of negative emission technologies and energy systems. Energy Environ. Sci. 12 (6), 1805–1817. doi:10.1039/C8EE03682A.
d'Amore, F., Bezzo, F., 2020. Optimizing the design of supply chains for carbon capture, utilization, and sequestration in europe: a preliminary assessment. Front. Energy Res. 8, 305. doi:10.3389/fenrg.2020.00190.
E3Modelling, 2018. PRIMES MODEL: Version 2018 Detailed model Description. E3Modelling.
Ecoinvent, 2020. Ecoinvent Data V. 3.6. Swiss Centre for Life Cycle Inventories. Ecoinvent.
Edenhofer, O.R., Pichs-Madruga, Y., Sokona, S., Kadner, J.C., Minx, S., Brunner, S., et al., 2014. Climate Change 2014: Mitigation of Climate Change. Contribution of Working Group III to the Fifth Assessment Report of the Intergovernmental Panel On Climate Change. Cambridge University Press, NY, USA Cam-bridge, United Kingdom and New York.
Escobar, N., Britz, W., 2021. Metrics on the sustainability of region-specific bioplastics production, considering global land use change effects. Resour. Conserv. Recycl. 167 (3), 105345. doi:10.1016/j.resconrec.2020.105345.
Escobar, N., Laibach, N., 2021. Sustainability check for bio-based technologies: a review of process-based and life cycle approaches. Renew. Sustain. Energy Rev. 135 (12), 110213. doi:10.1016/j.rser.2020.110213.
European Commission, 2011. Energy Roadmap 2050: Impact Assessmentand Scenario Analysis. European Commission.
European Commission, 2018. Top 20 Innovative Bio-Based Products. Publications Office of the European Union doi:10.2777/85805.
European Commission, 2020. The European Green Deal Investment Plan and Just Transition Mechanism Explained. European Commission.
Fasihi, M., Efimova, O., Breyer, C., 2019. Techno-economic assessment of CO_2 direct air capture plants. J. Clean. Prod. 224 (3), 957–980. doi:10.1016/j.jclepro.2019.03.086.
Finnveden, G., Nielsen, P.H., 1999. Long-term emissions from landfills should not be disregarded. Int. J. LCA 4 (3), 100. doi:10.1007/BF02979444.
Gabrielli, P., Gazzani, M., Mazzotti, M., 2020. The role of carbon capture and utilization, carbon capture and storage, and biomass to enable a net-zero-CO_2 emissions chemical industry. Ind. Eng. Chem. Res. 59 (15), 7033–7045. doi:10.1021/acs.iecr.9b06579.
Geres R., Kohn A., Lenz S.C., Ausfelder F., Bazzanella A., Möller A. Roadmap Chemie 2050: auf dem Weg zu einer treibhausgasneutralen chemischen Industrie in Deutschland eine Studie von DECHEMA und FutureCamp für den VCI, 2019. ISBN: 978-3-89746-223-6.
Geyer, R., Jambeck, J.R., Law, K.L., 2017. Production, use, and fate of all plastics ever made. Sci. Adv. 3 (7), e1700782. doi:10.1126/sciadv.1700782.
Gielen, D., Boshell, F., Saygin, D., Bazilian, M.D., Wagner, N., Gorini, R., 2019. The role of renewable energy in the global energy transformation. Energy Strategy Rev. 24 (6), 38–50. doi:10.1016/j.esr.2019.01.006.
Gielen, D., Newman, J., Patel, M.K., 2008. Reducing industrial energy use and CO_2 emissions: the role of materials science. MRS Bull. 33 (4), 471–477. doi:10.1557/mrs2008.92.
Gilbert, A., Sovacool, B.K., 2015. Emissions accounting for biomass energy with CCS. Nat. Clim Chang. 5 (6), 495–496. doi:10.1038/nclimate2633.
Global CCS Institute, 2021. Technology Readiness and Costs of CCS. Global CCS Institute.
Harper, A.B., Powell, T., Cox, P.M., House, J., Huntingford, C., Lenton, T.M., et al., 2018. Land-use emissions play a critical role in land-based mitigation for Paris climate targets. Nat. Commun. 9 (1), 2938. doi:10.1038/s41467-018-05340-z.
Heijungs, R., Suh, S., 2002. The Computational Structure of Life Cycle Assessment. Kluwer Acad. Publ, Dordrecht.
Hepburn, C., Adlen, E., Beddington, J., Carter, E.A., Fuss, S., Mac Dowell, N., et al., 2019. The technological and economic prospects for CO_2 utilization and removal. Nature 575 (7781), 87–97. doi:10.1038/s41586-019-1681-6.
Hoogwijk, M., Faaij, A., van den Broek, R., Berndes, G., Gielen, D., Turkenburg, W., 2003. Exploration of the ranges of the global potential of biomass for energy. Biomass Bioenergy 25 (2), 119–133. doi:10.1016/S0961-9534(02)00191-5.
ICIS. Supply and Demand Database, 2017. A Comparison of Induced Land-Use Change Emissions Estimates from Energy Crops. International Council on Clean Transportation.
International Energy Agency, 2013. Technology Roadmap: Energy and GHG Reductions in the Chemical Industry Via Catalytic Processes. International Energy Agency.
International Energy Agency, 2017a. Technology Roadmap: Delivering Sustainable Bioenergy. International Energy Agency.
International Energy Agency, 2018a. The Future of Petrochemicals: Towards more Sustainable Plastics and Fertilisers. International Energy Agency.
International Energy Agency, 2018b. World Energy Outlook 2018. International Energy Agency.
International Energy Agency, 2019. World Energy Investment 2019. IEA Publications.
International Energy Agency, 2020. Energy Technology Perspectives 2020. International Energy Agency.
International Energy Agency, International Renewable Energy Agency, 2017b. Perspectives for the Energy Transition: Investment Needs For a Low-Carbon Energy System. International Energy Agency, International Renewable Energy Agency.
International Energy Agency Bioenergy, 2007. Potential Contribution of Bioenergy to the World's Future Energy Demand. International Energy Agency Bioenergy.
Jens, C.M., Müller, L., Leonhard, K., Bardow, A., 2019. To Integrate or not to integrate—techno-economic and life cycle assessment of CO_2 capture and conversion to methyl formate using methanol. ACS Sustain. Chem. Eng. 575 (7), 12270–12280. doi:10.1021/acssuschemeng.9b01603.
Jiang, L., Gonzalez-Diaz, A., Ling-Chin, J., Malik, A., Roskilly, A.P., Smallbone, A.J., 2020. PEF plastic synthesized from industrial carbon dioxide and biowaste. Nat. Sustain. 3 (9), 761–767. doi:10.1038/s41893-020-0549-y.
Kätelhön, A., Bardow, A., Suh, S., 2016. Stochastic Technology choice model for consequential life cycle assessment. Environ. Sci. Technol. 50 (23), 12575–12583. doi:10.1021/acs.est.6b04270.
Kätelhön, A., Meys, R., Deutz, S., Suh, S., Bardow, A., 2019. Climate change mitigation potential of carbon capture and utilization in the chemical industry. Proc. Natl. Acad. Sci. USA 116 (23), 11187–11194. doi:10.1073/pnas.1821029116.
Khanna, M., Dhungana, B., Clifton-Brown, J., 2008. Costs of producing miscanthus and switchgrass for bioenergy in Illinois. Biomass Bioenergy 32 (6), 482–493. doi:10.1016/j.biombioe.2007.11.003.
Klemeš J.J., van Fan Y., Jiang P. Plastics: friends or foes? The circularity and plastic waste footprint. Energy Sources Part A Recovery Util. Environ. Eff. 2021;43(13):1549–65. 10.1080/15567036.2020.1801906.
Kühner, S.BioBoost, 2013. Biomass based Energy Intermediates Boosting Biofuel production: Deliverable Feedstock Costs. BioBoost.
Laing, T., Sato, M., Grubb, M., Comberti, C., 2014. The effects and side-effects of the EU emissions trading scheme. WIREs Clim. Chang. 5 (4), 509–519. doi:10.1002/wcc.283.
Lau, W.W.Y., Shiran, Y., Bailey, R.M., Cook, E., Stuchtey, M.R., Koskella, J., et al., 2020. Evaluating scenarios toward zero plastic pollution. Science 369 (6510), 1455–1461. doi:10.1126/science.aba9475, New York, N.Y..
Lebling, K., McQueen, N., Pisciotta, M., Wilcox, J., 2021. Direct Air Capture: Resource Considerations and Costs for Carbon Removal. World Resources Institute.
Lee, S.Y., Kim, H.U., Chae, T.U., Cho, J.S., Kim, J.W., Shin, J.H., et al., 2019. A comprehensive metabolic map for production of bio-based chemicals. Nat. Catal. 2 (1), 18–33. doi:10.1038/s41929-018-0212-4.
Lewandowski, I., Clifton-Brown, J., Kiesel, A., Hastings, A., Iqbal, Y., 2018. Miscanthus. In: Perennial Grasses For Bioenergy and Bioproducts. Elsevier, pp. 35–59.
Loulou, R., Goldstein, G., Kanudia, A., Lettila, A., Remme, U., 2016. Documentation for the TIMES Model: Part I. Energy Technology Systems Analysis Programme.
Material Economics, 2019. Industrial Transformation 2050 - Pathways to Net-Zero Emissions from EU Heavy Industry. Material Economics.
McCalmont, J.P., Hastings, A., McNamara, N.P., Richter, G.M., Robson, P., Donnison, I.S., et al., 2017. Environmental costs and benefits of growing Miscanthus for bioenergy in the UK. Glob. Chang. Biol. Bioenergy 9 (3), 489–507. doi:10.1111/gcbb.12294.
McCollum, D.L., Zhou, W., Bertram, C., Boer, H.S., de Bosetti, V., Busch, S., et al., 2018. Energy investment needs for fulfilling the Paris agreement and achieving the sustainable development goals. Nat. Energy 3 (7), 589–599. doi:10.1038/s41560-018-0179-z.

Meys, R., Kätelhön, A., Bachmann, M., Winter, B., Zibunas, C., Suh, S., et al., 2021. Achieving net-zero greenhouse gas emission plastics by a circular carbon economy. Science 374 (6563), 71–76. doi:10.1126/science.abg9853, New York, N.Y..

Mohammadi, M., Jämsä-Jounela, S.L., Harjunkoski, I, 2019. Optimal planning of municipal solid waste management systems in an integrated supply chain network. Comput. Chem. Eng. 123 (1), 155–169. doi:10.1016/j.compchemeng.2018.12.022.

Ögmundarson, Ó., Herrgård, M.J., Forster, J., Hauschild, M.Z., Fantke, P., 2020. Addressing environmental sustainability of biochemicals. Nat. Sustain. 3 (3), 167–174. doi:10.1038/s41893-019-0442-8.

Pawelzik, P., Carus, M., Hotchkiss, J., Narayan, R., Selke, S., Wellisch, M., et al., 2013. Critical aspects in the life cycle assessment (LCA) of bio-based materials – Reviewing methodologies and deriving recommendations. Resour. Conserv. Recycl. 73 (3–4), 211–228. doi:10.1016/j.resconrec.2013.02.006.

PlasticsEurope. Plastics – the Facts, 2018. An Analysis of European plastics production, Demand and Waste Data 2018. PlasticsEurope.

Quantis, 2020. Chemical Recycling: Greenhouse Gas Emission Reduction Potential of an Emerging Waste Management Route. Quantis.

Rahimi, A., García, J.M., 2017. Chemical recycling of waste plastics for new materials production. Nat. Rev. Chem. 1 (6), 409. doi:10.1038/s41570-017-0046.

Raven P., Berry S., Cramer W. Letter regarding use of forests for bioenergy (February 11, 2021), 2021. https://www.woodwellclimate.org/letter-regarding-use-of-forests-for-bioenergy/ (accessed April 15, 2021).

Ricke, K., Drouet, L., Caldeira, K., Tavoni, M., 2018. Country-level social cost of carbon. Nat. Clim. Chang. 8 (10), 895–900. doi:10.1038/s41558-018-0282-y.

Ritchie H., Roser M. Our World in Data: emissions by sector, 2021. https://ourworldindata.org/emissions-by-sector (accessed April 15, 2021).

Sanchez, D.L., Nelson, J.H., Johnston, J., Mileva, A., Kammen, D.M., 2015a. Biomass enables the transition to a carbon-negative power system across western North America. Nat. Clim. Chang. 5 (3), 230–234. doi:10.1038/nclimate2488.

Sanchez, D.L., Nelson, J.H., Johnston, J., Mileva, A., Kammen, D.M., 2015b. Reply to 'emissions accounting for biomass energy with CCS'. Nat. Clim. Chang. 5 (6), 496. doi:10.1038/nclimate2634.

Schmidt, T.S., 2014. Low-carbon investment risks and de-risking. Nat. Clim. Chang. 4 (4), 237–239. doi:10.1038/nclimate2112.

Schneider, C., Saurat, M., 2020. Simulating geographically distributed production networks of a climate neutral European petrochemical industry. In: Proceedings of the ECEEE Industrial Summer Study Industrial Efficiency 2020: Decarbonise industry!.

Searchinger, T., Heimlich, R., Houghton, R.A., Dong, F., Elobeid, A., Fabiosa, J., et al., 2008. Use of U.S. croplands for biofuels increases greenhouse gases through emissions from land-use change. Science 319 (5867), 1238–1240. doi:10.1126/science.1151861, New York, N.Y..

Seto, K.C., Davis, S.J., Mitchell, R.B., Stokes, E.C., Unruh, G., Ürge-Vorsatz, D., 2016. Carbon lock-in: types, causes, and policy implications. Annu. Rev. Environ. Resour. 41 (1), 425–452. doi:10.1146/annurev-environ-110615-085934.

Stegmann, P., Londo, M., Junginger, M., 2020. The circular bioeconomy: its elements and role in European bioeconomy clusters. Resour. Conserv. Recycl. X 6 (3), 100029. doi:10.1016/j.rcrx.2019.100029.

Wiloso, E.I., Heijungs, R., Huppes, G., Fang, K., 2016. Effect of biogenic carbon inventory on the life cycle assessment of bioenergy: challenges to the neutrality assumption. J. Clean. Prod. 125 (5), 78–85. doi:10.1016/j.jclepro.2016.03.096.

World Economic Forum, Ellen MacArthur Foundation and McKinsey & Company. The New Plastics Economy – Rethinking the future of plastics 2016. https://ellenmacarthurfoundation.org/the-new-plastics-economy-rethinking-the-future-of-plastics (accessed April 15, 2021)

Zhang, S., Jiang, S.F., Huang, B.C., Shen, X.C., Chen, W.J., Zhou, T.P., et al., 2020. Sustainable production of value-added carbon nanomaterials from biomass pyrolysis. Nat. Sustain. 3 (9), 753–760. doi:10.1038/s41893-020-0538-1.

Zheng, J., Suh, S., 2019. Strategies to reduce the global carbon footprint of plastics. Nat. Clim. Chang. 9 (5), 374–378. doi:10.1038/s41558-019-0459-z.