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Environmental and economic assessment of CO_2-based value chains for a circular carbon use in consumer products

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ABSTRACT

The currently fossil-based production and highly linear use of polymer products generates significant amounts of CO_2 emissions and irretrievably wastes resources. To address these challenges, effective and competitive technologies are required to enhance the circularity of carbon use. In this study economic and environmental effects of the use of CO_2 as carbon source for polymer products such as packaging, construction material or medical products are analyzed. Thereby, the whole value chain, from the CO_2 source to the market-ready product is considered. Material flow cost accounting is combined with environmental indicators to assess 28 possible CO_2-based value chains. Data envelopment analysis (DEA) is used to compare the alternatives and to identify the most eco-efficient examples considering production costs, CO_2-emissions, energy demand and fossil carbon use. In all cases, a significant reduction of CO_2-emissions is achieved compared to the conventional alternative. For subsequently produced consumer products with a high value, the additional costs for CO_2-based value chains are between 0.7 – 4% in the status quo and 0.1 – 1% in a future scenario which enables a market entrance for CO_2-based products with comparably small price premiums. Considering the studied assessment indicators, the use of CO_2 can already lead to the same or a similar overall performance compared to fossil-based production. The choice of the right product and value chain set up is decisive, with economies of scale playing a significant role. The results further show that costs and benefits are currently imbalanced along the value chain, wherefore an effective cooperation is key to achieve market readiness.

1. Introduction

The amount and the way how fossil hydrocarbons are consumed in the global economy raise multiple problems. Most importantly, the largest share of global Green House Gas (GHG) emissions origins from burning fossil fuels, which in turn is the reason for human-made climate change (IPCC 2014). In addition, the mainly linear use of fossil resources leads to their irretrievable depletion (IRP, 2019). Most recently, supply bottlenecks caused by disrupted supply chains due to global or regional crises led to significant price peaks for oil-based products and clearly showed the economic risks of supply shortages (S&P-Global, 2021). Thus, new options of hydrocarbon production and use must be developed which avoid CO_2-emissions, enable a circular use of resources, and therefore contribute to a circular economy.

For the chemical industry in general and specifically to produce organic chemicals, this requires a decoupling of the current material and energy supply which both use fossil hydrocarbons as the main input (Kaiser and Bringezu 2020). On a global scale, this leads to a direct emission volume of 0.7 Gt CO_2-eq. per year (IEA 2021), for the production processes alone. Beside these direct energy and process related emissions during the production of chemicals and polymers, about the same amount of emissions takes place in the end-of-life (EoL) phase of material carbon (Schmidt et al., 2021). For example, in the German chemical industry, 56 out of 112 Mt CO_2-eq. per year are emissions which originate from waste management of polymer materials based on carbon from fossil sources (Geres et al., 2019; UBA 2018). While alternative technologies for the provision of energy enable the substitu tion of hydrocarbons and therefore also the avoidance of the related CO_2-emissions (Bazzanella and Ausfelder, 2017), the EoL emissions which originate from the material use of fossil carbon are harder to abate. Here, the carbon cannot be substituted but must be won from different sources.

One promising option are *Carbon Dioxide Capture and Utilization* (CCU) technologies, i.e., the CO_2-based production of chemicals. CO_2 is

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used as a carbon source in combination with water and electricity which enables a fossil-free production for a broad range of organic chemicals (Mikkelsen et al., 2010). The required CO_2 can be sourced from different point sources as well as the atmosphere (Von der Assen et al. 2016). According to Kaiser and Bringezu (2020) and Müller et al. (2020) the use of only unavoidable and long-term available point-sources such as cement or biogas upgrading plants alone could suffice the carbon demand of the chemical industry in the future. In addition, the technical feasibility to produce a major share of the currently produced base chemicals on the basis of CO_2 has been demonstrated while the underlying technologies provide a high technological readiness level (Geres et al., 2019; Bazzanella, 2017). The climate impact of the production of chemicals and polymers could be significantly reduced, if the required electricity is won from renewable sources (Hoppe et al., 2017; Sternberg et al., 2017; Ravikumar et al., 2021). Thus, a broad defossilization of the global chemical industry via CCU technologies would significantly reduce CO_2 emissions but require large amounts of renewable electricity (Kätelhön et al., 2019).

Another challenge for the production of CO_2-based chemicals is the economic viability. Recent studies showed that for the production of base chemicals, e.g., methanol, competitiveness is not achieved at the moment but could be realized in the near future (Hank et al., 2018; Hoppe et al., 2018). The main cost driver are the costs for hydrogen via electrolysis and thus the costs for electricity and electrolyzer plants (Hank et al., 2020). The right location plays a significant role with wind-based locations outperforming Photovoltaic-based locations due to higher plant utilization (Kaiser et al., 2021). Furthermore, the respective rate of capital costs has a significant impact as well, wherefore production locations in northern Europe and South America are most likely to reach competitiveness in the near future. The focus on merely the production costs of base chemicals, however, leaves out the economic assessment from a value chain wide perspective as well as the possible contribution of CCU technologies to a circular economy. The latter is created by turning the mainly linear material flows into closed-loop value chains (Schenkel et al., 2015). This is especially necessary for the chemical and polymer sector, where less than 10% of the carbon input originates from secondary sources (Kaiser and Bringezu 2020). The necessary transformation requires the development of new business models in combination with a reshaping of supply chains and value creation (Lüdeke-Freund et al., 2019; Karayılan et al., 2021). The production of CO_2-based polymers could depict such a new business model which is based on a circular use of carbon. Their use in consumer products offers a higher value creation than the production of base chemicals since the share of feedstock costs on total costs decreases with increasing value creation and thus also the additional costs per product (Wilting and Hanemaaijer 2014).

At the moment, CO_2-based chemical production shows a trade-off between climate mitigation and other environmental impact categories as well as cost efficiency. Hence, multiple assessment indicators are necessary for a thorough assessment. A sound combination of environmental and economic aspects within one analysis, however, can be difficult since the used indicators are not always comparable. To solve this problem and to identify the best overall alternative, suitable methods for multi criteria analysis are necessary (Zanghelini et al., 2018). In recent literature, sophisticated weighting methods were developed and used to compare CO_2-based chemicals, e.g. Chauvy et al. (2019) or Pacheco et al. (2021). However, despite their complexity, the methods still involve a certain level of subjectivity to choose the respective category weights. To further eliminate subjectivity in the comparison, the approach of *Data Envelopment Analysis* (DEA) can be used. The method was developed by Charnes et al. (1978) and is applied to compare environmental with economic assessment indicators (Mardani et al., 2018; Zhou et al., 2018; Song et al., 2012) or to calculate eco-efficiency values (Thies et al., 2019) without the exogenous determination of weights or priorities. Nevertheless, the application of DEA also shows some drawbacks. For example, to generate valid results a minimum number of alternatives is required, and the comparability of the compared objects must be thoroughly examined and assured with the help of suitable criteria. In addition, the DEA results do not show a clear priority sequence (Kerpen 2016; Liang et al., 2017). Practical examples for the application of DEA are the comparison of manufacturing sectors (Egilmez et al., 2013), supply chain management strategies (Gold et al., 2017) or the eco-efficiency of industrial parks (Hu et al., 2019; Wang et al., 2021). In the context of CCU technologies, the method has been used to compare solvents for CO_2-capture (Limleamthong et al., 2016) but it has not yet been applied to calculate eco-efficiencies of CO_2-based products.

Based on the identified research gaps, this article addresses the questions of how CO_2-based polymer production can be characterized as a circular economy business model (CEBM) and what the economic and environmental characteristics of a complete CO_2-based value chain for consumer products could be. Thereby, it combines the analysis of several case examples for CO_2-based value chains for status quo conditions and a future scenario with a DEA to identify promising constellations for a market introduction.

2. Methods and data

To answer the research question, representative case examples for possible CO_2-based value chains are identified, modelled, and assessed using suitable indicators. In the following section the applied research methods, models and case examples are described in detail.

2.1. Case examples

To identify representative case examples for consumer products the following categories were used: *polymer type; polymer content*, i.e., the mass share of polymer in the consumer product; *functional value of the polymer*, i.e., the share of product value which originates from the polymer in the product, expressed by the share of polymer production costs in the total production costs; *sector of product application*. The availability of detailed data for the polymer content of the products, e.g., via product information sheets, was another factor in the selection process. The analyzed case examples (Table 1) stem from six main application sectors for polymers (Lindner and Schmitt, 2018). As polymer types, three mass polymers (Polyethylene (PE), Polypropylene (PP) and Polyvinylchloride (PVC)) and one technical polymer (Polyoxymethylene) (POM) were selected. The polymer content as well as the share of polymer production costs cover a broad range of possible combinations. Thereby, the share of polymer costs was calculated for each case example in the following way. First, the polymer content was

Table 1
Description of the analyzed case examples. (HDPE = High Density Polyethylene, LDPE = Low Density Polyethylene, PP = Polypropylene, PVC = Polyvinylchloride, POM = Polyoxymethylene).

Product	Description	Application Sector	Polymer Type	Polymer Content (mass%)	Share of Polymer Costs on Total Production Costs
P1	Bottle for Disinfection Gel	Packaging	HDPE	12%	0.6%
P2	Bubble Warp	Packaging	LDPE	100%	19%
P3	Marker Body	Home Appliance	PP	18%	0.3%
P4	Medical Syringe	Health Care	PP	70%	1.4%
P5	Cable Mantle	Electronics	PVC	38%	4%
P6	Pipe	Construction	PVC	100%	2.9%
P7	Cog Wheel	Machinery	POM	100%	1%

determined with the help of product information sheets and own calculations. Second, the amount of polymer needed was combined with production costs for the polymers. Third, the costs for the required polymers were compared to the production costs of the consumer product. The value chain for the polymer production was modeled for the fossil-based and four CO_2-based alternatives, considering different CO_2-sources (Cement, Waste Incineration, and Biogas Plant, Direct Air Capture (DAC)). The CO_2 sources are differentiated because they provide different CO_2 concentrations, specific emission volumes and capture costs. In total, 28 CO_2-based values chains and 7 fossil-based values chains were considered for the analysis.

2.2. Material flow cost accounting and data envelopment analysis

The systemic environmental and economic analysis of a value chain requires the combined modeling of material, energy, and cash flows. Therefore, a material flow cost accounting (MFCA) analysis was conducted in accordance with DIN 14051 (DIN-EN-ISO, 2011) and complemented with environmental assessment indicators. This method has been demonstrated on organizational and value-chain level, e.g., to reduce costs related to material losses (Walz and Guenther 2021; Christ and Burritt 2015), or to compare different regional recycling networks (Walther 2010). Thus, it is a suitable tool to analyze and compare CO_2-based value chains from an environmental and economic perspective.

The results of the flow analysis are further used to calculate the assessment indicators. These indicators were chosen with respect to the effects of a feedstock change for the chemical production, which is the main difference between fossil- and CO_2-based value chains. For their identification, recent LCA and economic assessment studies were used, e.g., Hoppe et al. (2018) or Kaiser et al. (2021) as well as relevant environmental targets. As main effects of a feedstock change the resulting CO_2-emission, the used carbon source, the energy requirement, and the production costs were identified. In addition, the reduction of CO_2-emissions and primary energy use as well as an increased use of secondary carbon are important targets for companies according to actual policies (European Commission 2021). Therefore, the *polymer related* CO_2-emissions, the *production costs*, the *fossil carbon input,* i.e., the amount of carbon which is won from fossil sources, and the *cumulative energy demand* were chosen as assessment indicators and calculated for each case example and value chain option.

For a further comparison of the results, DEA was applied. Thereby, each value chain was considered as a so-called *Decision-Making Unit* (DMU). The comparison is enabled by calculating and comparing the performance of all DMUs within an empirically determined technology area (Dyson et al., 2001). The technology area defines the technical capabilities of the DMUs in their entirety, while the performance of a single DMU shows how it utilizes these capabilities. To measure the performance of each DMU, a set of optimal weights for each input and output is determined. The weights are calculated endogenously by formulating and solving an optimization problem which considers all DMUs. To identify the most efficient DMUs, an efficiency score is calculated for every DMU using the specific set of optimal weights. As boundary condition, the maximum efficiency score is 1, i.e., 100%. If one DMU shows an efficiency score of 1, it can be considered as relatively efficient compared to the other DMUs and thereby lies on the efficiency frontier. Vice versa, if one DMU shows a score below 1 despite the use of an optimal weighting set, this means that there is at least one other DMU which is more efficient.

As DEA model, an input oriented CCR (Charnes, Cooper, and Rhodes) model was chosen for the analysis. The described assessment indicators are considered as input variables and combined with the revenue per consumer product as output variable. These variables represent the main factors to describe the regarded transformation process for each value chain. CO_2-emissions are counted as an input even though they are a physical output since they represent an undesirable output which uses the capacity of the environment for its disposal (Dakpo et al., 2016). In other words, every ton of emitted CO_2 lowers the remaining carbon budget wherefore it can be seen as a scarce good. The DMUs can be regarded as comparable according to Kerpen (2016) and Dyson et al. (2001) since they fulfill the same function, namely to generate revenue, and thereby use the same resources and similar technologies in the same time period. The number of 35 DMUs fulfills the criteria for the minimum amount of DMUs necessary to achieve a reasonable level of discrimination according to Dyson et al. (2001) and Cooper (2007). Constant returns to scale were assumed to show the effect of different specific emission volumes, i.e., production scales, on the performance of one value chain. In a model with variable returns to scale, differences in scale are leveled within the model to exclude them from the efficiency calculation. Therefore, a scaling effect would not be visible or distorted. The relative performance of each DMU is shown by the respective efficiency score which sets the studied environmental and economic indicators into relation.

$$Efficiency\ score_{Product\ i} = \frac{weighted\ Revenue_{Product\ i}}{\sum weighted\ Inputs_{Product\ i}}$$

Solving the DEA problem identifies those value chains which produce one unit of revenue with the most efficient use of the available resources. The efficiency score can further be considered as eco-efficiency, if one of the environmental indicators is reduced, e.g., via the avoidance of CO_2-emissions, compared to the fossil-based processes. The latter represent the prevailing alternatives and serve as a benchmark for the new value chains. They cannot be considered as eco-efficient due to the inherent use of fossil resources and the accompanied environmental problems. The modeling and solving of the DEA problem was done with the open source software *OSDEA (Version 0.2)* as well as *R (Version 4.1.2)* using the *Benchmark and Frontier Analysis Package* from Bogetoft and Otto, 2020. The formal model can be found in the SI-1.

To classify CO_2-based value chains as CEBM and to compare them with existing regulation schemes, existing classification schemes from the literature were used. Further information can be found in SI-2 while the results are presented in Section 3 of this article.

2.3. System description

To analyze and compare the value chains, an MFCA was conducted for each alternative. All necessary production processes, i.e., the CO_2 capture and electrolysis (for CO_2-based alternatives) or naphtha production (fossil-based alternatives), the production of chemicals, monomers, polymers, and the consumer products are regarded as system elements, as well as the product specific sales market and the EoL phase. Even though the last two elements do not belong to the value chain, they are important to calculate the input of the operative cash flow in form of market revenues and to achieve an equal carbon balance by also considering EoL emissions (Fig. 1). The functional unit is defined as one produced unit of a consumer product. The carbon, energy, and cash flows of the system are used to calculate the assessment indicators per functional unit. Due to overall promising location factors, such as the availability of CO_2 sources, chemical and polymer industries as well as markets for the consumer products, the analysis focuses on value chains located in Germany. As background data, e.g., for the provision of energy from the grid or fossil feedstock prices, actual data for Germany was considered. Detailed process data for the fore- and background can be found in SI-3.

The study focuses on the effect of CO_2-utilization as carbon source for polymer production. Therefore, the production of further ingredients or components of the products were not included, since they are not altered, and their modeling is not necessary to measure the effects of different polymer production technologies. The necessary production of H_2 is assumed as a stand-alone process for which the use of electricity from renewable sources is crucial to reach an overall favorable ecological performance for CO_2-based polymer production (Hoppe et al., 2017;

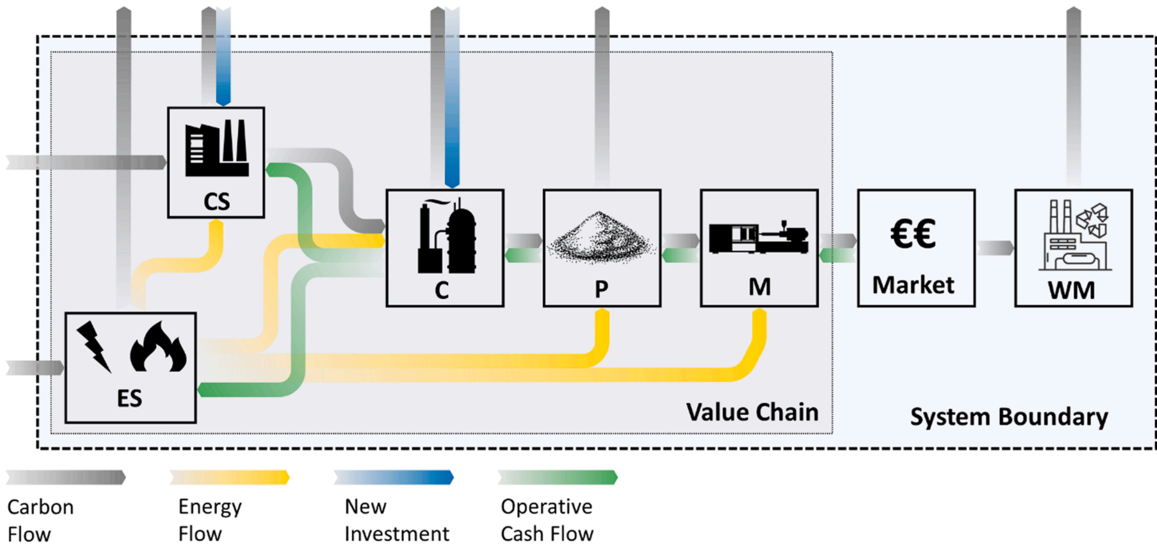

Fig. 1. System elements, flows and boundary for the material flow cost-accounting (CS = Carbon Source, ES = Energy Source, C = Chemical Production, *P* = Polymer Production, *M* = Product Manufacturing, WM = Waste Management).

Sternberg et al., 2017). Thus, energy provision via wind electricity was assumed. The wind electricity could be provided via the grid in combination with purchase power agreements or via additionally constructed capacity. Both strategies are currently pursued by companies in Germany to get exclusive access to renewable electricity (Axpo 2022; BASF 2021). Because there is a lack of transport infrastructure for CO_2, H_2, and some of the monomers, it was assumed that gaseous products are further processed onsite. Thereby, the necessary processes (CO_2-capture, methanol, and monomer synthesis) need to be integrated in already existing plants, wherefore the required process energy is provided by the grid. For the produced CO_2-based methanol and polymers, a transport to further processing plants via road is assumed. Thus, the specific emission volume of the considered CO_2-source determines the throughput of the value chain. As EoL process, waste incineration was considered.

The production costs for CO_2-based value chains were calculated using data from the recent literature for the plant costs and scales for every production step. The production costs for the fossil-based chemicals, polymers and consumer products were approximated using average net market prices. It was assumed, that the net market prices include a margin of 10%, which was subtracted out to calculate the difference in production costs for polymer production (see SI-3 for detailed cost data). The cost differences between fossil and CO_2-based alternatives for the consumer products were calculated by comparing the production costs for the respective monomers (ethylene, formaldehyde, and propylene). It was further assumed that the CO_2-based monomers are used as a drop-in and that the cost difference would be passed through the value chain to the consumer product.

Table 2
Description of the different emission scopes used to classify the CO_2 emissions of each system element. The classification is based on WRI and WBCSD (2011), WRI, and WBCSD (2015).

Emission scope	Description	Application in this study
Scope 1	Emissions from sources that are owned or controlled by a company.	Direct emissions which are caused by a system element.
Scope 2	Emissions from the generation of purchased or acquired electricity, steam, or heating.	Emissions which are caused by the energy supplier for one system element.
Scope 3	All other indirect emissions that occur in the value chain.	Emissions from other system elements in the value chain (except the energy supplier)

The CO_2-emissions caused by the carbon and energy flows into and within the system are classified for each system element (Table 2). To compare the potential environmental benefits with the potentially higher production costs, CO_2-abatement costs as well as carbon circulation costs are calculated. The former is defined as the additional costs per avoided t of CO_2 emissions and focusses on the costs for emission avoidance. The latter expresses the additional costs required to recycle one ton of carbon, i.e., to substitute one ton of fossil carbon as primary material. Both indicators give information about the cost effectiveness of a CO_2-based value chain with respect to the environmental benefits and enable a comparison to other technologies aiming at emission abatement or carbon recycling. The calculation formulars can be found in SI-3.

To explicitly show the structure of the cash flows on the value chain-level, one exemplary value chain with a production capacity for CO_2-based methanol production of 100 kt/a was considered. This capacity is derived from the largest existing CO_2-based methanol production plant (CRI 2020). Based on the emission volumes considered in this study, the respective CO_2-demand of 147 kt per year could be supplied by a cement or waste incineration plant. A cement plant was chosen as CO_2-source because it offers lower capture costs. This supply volume of CO_2 would enable the production of 38 (PE and PP), 65 (POM) or 71 kt (PVC) CO_2-based polymer per year. This corresponds to 2% (PE and PP), 5% (PVC) or 22% (POM) of the domestic production volume in 2020 and 23% (PE) 31% (PVC), 67% (PP) or 149% (POM) of the average yearly production volume for a respective polymer producer in Germany (Destatis 2020).

2.4. Scenario analysis

To factor in future developments, the different value chains were analyzed for the status quo as well as for the years 2030 and 2050 with the help of a scenario analysis. The input parameters with a relatively high influence on the results were identified via a sensitivity analysis and altered according to a possible development described in the literature. The described development path represents a progressive development and illustrates how the performance of CO_2-based value chains could develop in a best-case scenario for cost parameters and the energy grids in Germany (Table 3). For the latter, climate neutrality is assumed for 2050. Currently, CCU technologies for chemical production are not creditable in emission trading schemes. In the scenario, it was assumed that the captured CO_2 is credited in the emission trading scheme by

Table 3
Assumed development for the scenario parameters. For the electricity grid, climate neutrality was assumed in 2050 (FLH = Full load hours, GWI = Global Warming Impact).

Parameter	2020	2030	2050	Sources/Assumptions
GWI Electricity [kg CO_2-eq./MJ]	0.1	0.01	0	(UBA 2016; Prognos et al. 2021)
GWI Heat [kg CO_2-eq./MJ]	0.06	0.004 (Use of heat pumps)	0 (Use of heat pumps)	(BAFA 2020) Coefficient for Heat Pumps: 3 (2030), 5 (2050) according to European Copper Institute (2018)
Electricity Costs (Grid Mix) [€/MJ]	0.05	0.05	0.05	(DENA 2018)
Electricity Costs (Wind Electricity) [€/MJ]	0.023	0.022	0.018	(Fraunhofer ISE 2021) Including transmission costs based on (DENA 2018)
Heat Costs [€/MJ]	0.012	0.011	0.01	Own calculation based on prices for fossil-feedstock or electricity
Polymer Costs [yearly change]	–	+1% (I) −0.3% (D)	+1% (I) −0.3% (D)	Calculation based on an increasing (I) and decreasing (D) oil price scenario from (IEA 2020b). Based on market data for monomers and polymers it was estimated that an average of 30% of the oil price deviation are passed on to polymer prices.
System EfficiencyElectrolyzer	67%	69%	74%	(Merten et al., 2020)
Electrolyzer Capex [M€/MW]	1.4	0.7	0.3	
Stack Lifetime [FLH]	60,000	78,000	105,000	(NOW, 2018)
Runtime [FLH/a]	3,000	5,000	8,000	The expansion of renewable energies in the grid allows a decoupling of the electrolyzer from site specific production curves and thereby increases the yearly runtime.
H_2-demand MeOH Synthesis [kg H_2/kg MeOH]	0.198	0.195	0.188	Gradual decline to the theoretical minimum in 2050.
MeOH-demand MTO [kg H_2/kg MeOH]	2.57	2.48	2.28	Gradual decline to the theoretical minimum in 2050.
CO2-Certificates [€/t CO_2]	–	85	255	2030: (Ewa Krukowska, 2021) 2050: Linear, yearly increase based on the assumed development between 2020 and 2030.

2030. The saved certificate costs for the otherwise emitted CO_2 emissions are not accredited to the CO_2-emitter but the base chemical producer who delivers the service of using the CO_2. At the same time, emission costs are added to every downstream process with CO_2-emissions (including EoL) to guarantee that every emission is accounted for. Due to the mentioned uncertainties for the oil price development, the scenario was further differentiated between increasing (I) and decreasing (D) oil prices. The effect of oil price fluctuations on polymer costs was estimated based on historical market data (2010 – 2020) for crude oil and the polymer types regarded in this article .For the plant costs of CO_2 capture, a reduction of 30% until 2030 was considered according to (IEA 2020a).

3. Results

3.1. CO_2 emissions and energy requirement

The system wide CO_2 emissions can be significantly reduced for every product (Fig. 2). The absolute emission volume as well as the relative reduction mainly depends on the chosen CO_2-source. For biogas upgrading, cement and waste incineration plants a significant reduction can be achieved, while the use of DAC would lead to only minor reductions in the status quo. The highest reduction can be achieved using plants for biogas upgrading, due to the high CO_2-content in the feed gas. The used polymer type and the respective production process are decisive for the reduction potential as well. For PE and PP, a reduction of 73% is possible, while the maximum values for PVC and POM are 61% and 56% . To produce POM, the impact of the CO_2-source is lower than for the other polymers, due to the more energy intensive polymerization step which leads to a higher impact of energy related emissions compared to the other polymers. Furthermore, the CO_2-based methanol is used as a drop-in, while for the other polymer types, the required ethylene or propylene is provided by an exothermal process substituting the endothermal and energy intensive steam-cracking process of naphtha which is used for the fossil-based production.

The CO_2 balances of the value chains show in more detail, how the resulting emission reductions for CO_2-based processes are achieved (Fig. 3). Within the first two production steps, i.e., the provision of feedstock, the overall emissions savings of the value chain are caused via capturing and using CO_2 in form of negative emissions. For the following production steps, the CO_2-balances are similar to the fossil-based production. Even though the captured CO_2 is ultimately released back into the atmosphere via waste incineration, wherefore CO_2-based polymers must not be considered as carbon sinks in general, the system wide emissions are significantly reduced due to the substitution of fossil feedstock by captured CO_2. In both cases, the majority of polymer related emissions is caused in the EoL stage , but the total amount depends on the used carbon source. Hence, for producers of polymers and polymer products the cause and the release of the largest share of CO_2-emissions related to their products lie in the up (cause) and downstream (release) processes and therefore out of their organizational boundaries.

In contrast to the CO_2-emissions, the CO_2-based value chains require a higher cumulative energy demand than the fossil-based alternatives (Table 4). Instead of extracting energy-rich molecules from geological reservoirs by using fossil fuels, the energy must now be provided by renewable sources and transformed via multiple processes, which involve energy losses (Fig. 3). For example, a third of the required energy is lost in the electrolyzing step alone. For products made of POM, the additional energy demand is significantly lower, because of the comparably high energy intensity of the fossil-based feedstock production, i.e., methanol based on natural gas. It is noteworthy, that the CO_2-source has a significant impact on the cumulative energy demand due to the different CO_2-concentrations in the input gas. Using DAC as carbon source, the additional energy requirement is more than two times higher than using a biogas upgrading plant. The results for the process specific emissions and energy requirements can be found in the SI-4.

3.2. Economics

While the single system elements of the examined CO_2-based value chains follow a linear business model, the value chain as a whole can be regarded as a Circular Economy Business Modell (CEBM) which fits to the pattern of a recycling business model according to Lüdeke-Freund et al. (2019). Compared to a fossil-based value chain, emission volumes and primary material use are reduced with the help of closed material loops. The provision of secondary carbon and the reduction of CO_2-emissions depict valuable services, which are generated in addition to the mere provision of a product. Instead of the production of oil, the value creation process starts with capturing CO_2 which will otherwise be (point sources) or was already (DAC) emitted into the atmosphere. Therefore, carbon is recycled while fossil resources are kept in the ground. The additional value can be captured by achieving a price premium, i.e., a higher sales price than the fossil-based alternative, at the consumer market or by recognizing the provided services, e.g., in

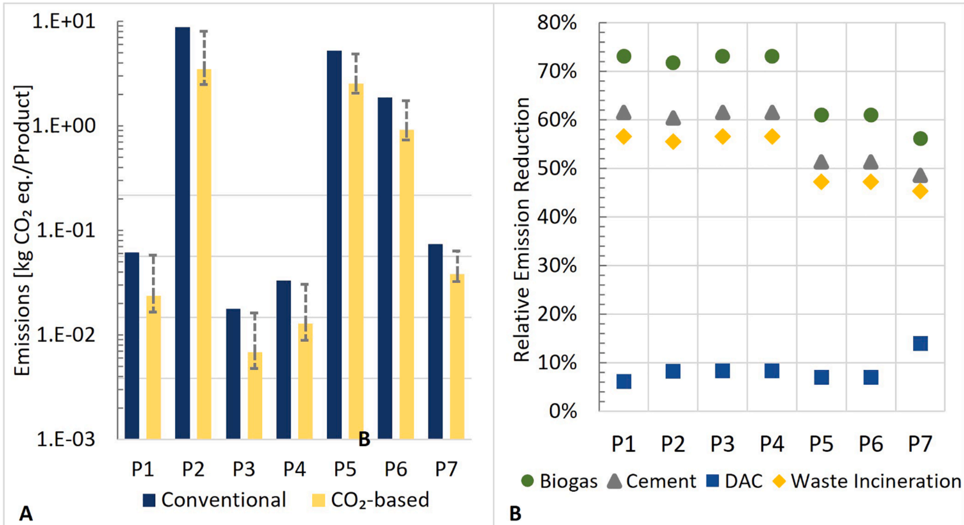

Fig. 2. A) Comparison of the system wide polymer related CO_2 emissions for a value chain using a cement plant as CO_2 source with a fossil-based value chain. The differences between the CO_2-sources are displayed with ranges. **B)** Relative Emission reduction potential compared to the fossil-based alternative. The characterization of the different products (P1-P7) can be found in Table 1.

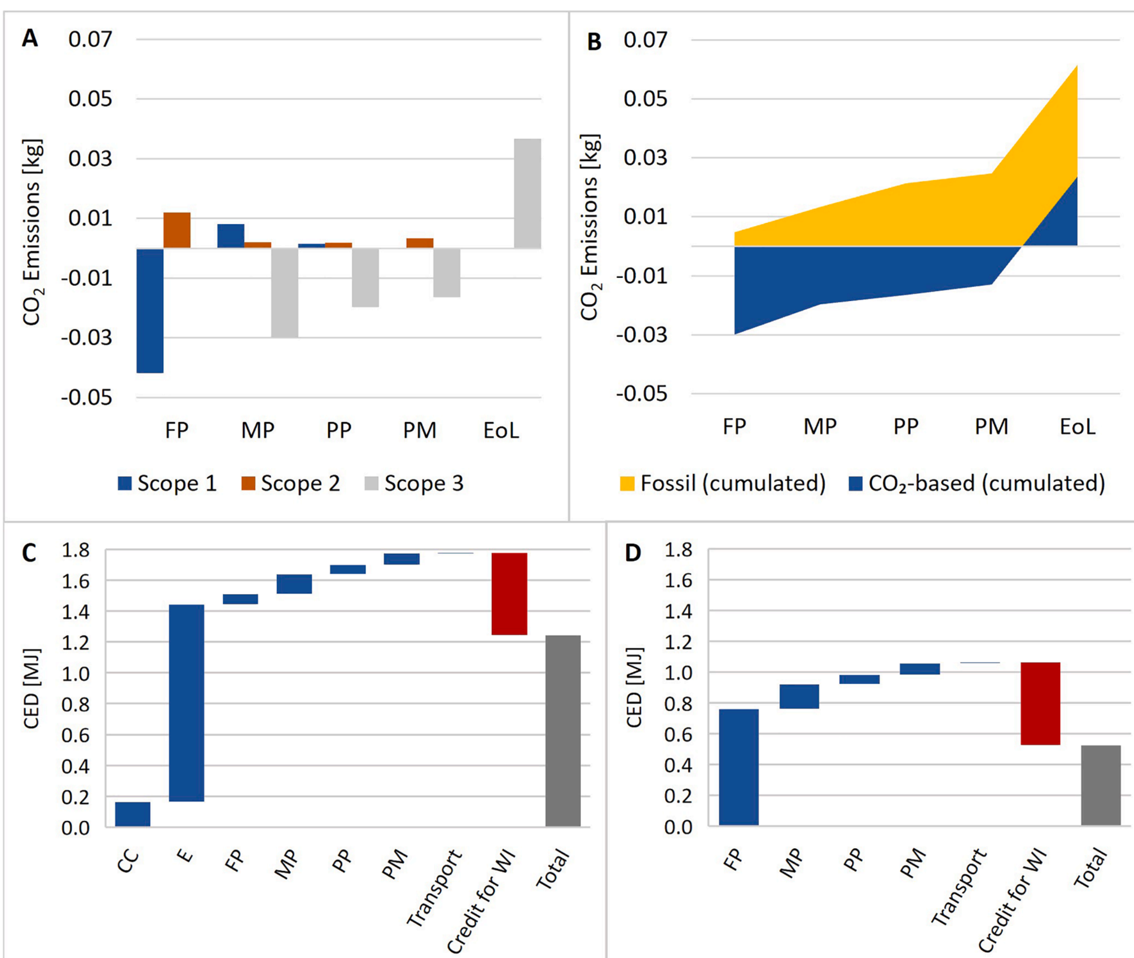

Fig. 3. A) Process specific CO_2 balances for a CO_2-based value chain. **B)** Comparison of cumulated CO_2-emissions of a fossil and CO_2-based value chain. Cumulative Energy Demand (CED) for **C)** a CO_2-based and **D)** a fossil-based value chain. The value chains for Product 1 are used as example. For the CO_2-based value chain a cement plant was assumed as CO_2-source. (CC = Carbon Capture, *E* = Electrolysis, FP = Feedstock Production, MP = Monomer Production, PP = Polymer Production, PM = Product Manufacturing, EoL = End-of-life, WI = Waste Incineration).

Table 4
Increase in Cumulative Energy Demand for the CO_2-based alternatives, compared to the fossil-based production. The description of the different products can be found in Table 1. (DAC = Direct Air Capture).

CO_2-Source	CO_2 concentration in feed gas	P1	P2	P3	P4	P5	P6	P7
Cement	20%	141%	134%	137%	141%	227%	99%	31%
Waste Incineration	10%	155%	148%	151%	155%	249%	110%	36%
Biogas	45%	112%	107%	109%	112%	183%	79%	21%
DAC	0.04%	281%	268%	274%	281%	443%	198%	81%

emission pricing schemes or input quotas. Thereby, the creation of the additional value is proposed at the start of the value chain by substituting fossil carbon sources, while the value capture takes place at its end. At the same time, the current regulation falls short to acknowledge the functions of CO_2-based value chains. Therefore, the realization of a price premium is currently the only way to capture the additional value.

For all case examples, the production costs are higher than for those processes using fossil-based polymers. At the same time, the relative increases differ significantly (Fig. 4) with the choice of the product being more relevant for the price premium than the choice of the CO_2-source. For products with a comparably low functional value of the contained polymer (P1, P3, P4, P7) the mean cost increase lies between 0.7% – 4% using a cement plant as CO_2 source. For products with high functional value of the polymer (P2, P5, P6) the mean cost increase lies between 6% to 47% (Fig. 4). If higher or lower production costs are assumed for the conventional products, the relative increases differ accordingly without changing the main aspects of the results. In general, those value chains using a cement plant as CO_2-source show the lowest production costs for each product due to economies of scale, i.e., higher yearly emission volumes. The cost increase is 4% (Waste Incineration), 24% (Biogas) or 65% (DAC) higher for each product for the other CO_2-sources. The results for process specific costs can be found in the SI-4.

The CO_2-abatement costs range from 761 to 1049 €/$t_{CO_2\text{-avoided}}$ in the status quo. The differences can be explained by the CO_2-source and the polymer type. Because only polymer related emissions are considered in this study, the product specific CO_2-abatement costs do not differ between products if the same polymer type is used. As for the production costs, value chains using a cement plant as CO_2-source show the lowest CO_2-abatement costs. They offer the best ratio between additional costs and the avoided emissions due to the higher scale of the value chain in combination with the second lowest CO_2 capture costs. Even though a higher emission reduction and lower CO_2-capture costs can be achieved using a biogas plant, the comparably small scale of the value chain causes higher production costs which result in higher abatement costs. However, using a biogas plant shows better results than a waste incineration plant, despite the higher scale of the latter. For the polymer types, POM shows the best relation between CO_2-based and fossil-based production costs of 1.6, compared to 3.3 (PE), 3.5 (PP) and 2.8 (PVC). This partly compensates the higher emission reductions of PE and PP and leads to a different ranking for the minimum abatement costs than in case of the possible emission reduction: 761 (P7, POM), 1017 (P1 and P2, PE), 1034 (P5 and P6, PVC), 1049 €/$t_{CO2\text{-avoided}}$ (P3 and P4, PP). Therefore, the throughput of the value chain, the possible emission reduction and the different production costs for polymers play the most important role to determine the abatement costs for a CO_2-based value chain.

The results for carbon circulation costs show a slightly different picture. Beside the production costs, the efficiency of carbon use i.e., the carbon losses due to process inefficiencies, has an important impact. The polymer production processes show carbon losses of 12% (PE and PP), 21% (PVC) and 30% (POM). Therefore, products 1 and 2 show the lowest circulation costs of 3836, compared to 3958 (P3 and P4), 4384 (P7) and 4693 €/$t_{\text{carbon circulated}}$ (P5 and P6). In consequence, different products must be considered as the most cost-efficient case, depending on the pursued environmental goal. In case of CO_2-emissions reduction costs, products such as POM-based P7 might be chosen, while for carbon recycling products like PE-based P1 and P2 would be the more cost-efficient alternatives.

The analysis of the cash flows for the exemplary value chain shows the cost structure and sets the additional costs in relation to the potential market revenue (Fig. 4). On the one hand, the results show the necessary investment requirements between 40 (CO_2 capture) and 359 M€ (H_2-production), 504 M€ in total, for processes at the start of the value chain. In addition, operational expenditures from 9 (CO_2 capture) to 110 M€ (H_2-production) would arise per year. Within the production of CO_2-based chemicals, the H_2-production requires the highest share of investment (64%) and operational expenditures (58%). On the other hand, the provision of the CO_2-based feedstock does not require additional investment for the polymer producer and the product manufacturer. Nevertheless, it would lead to additional operational expenditures, i.e., material costs between 119 (POM) and 136 M€ (PP) per year to enable a cost-covering production for the feedstock suppliers, compared to the use of fossil-based feedstock. Depending on the produced polymer type and the respective product these additional costs are faced with possible revenues between 0.3 and 17 billion € per year. The assumed production volumes of polymers would possibly saturate the polymer demand if only one single product is assumed. For example, 3 billion plastic bottles or 11 billion medical syringes could be produced which corresponds to roughly 39% or 480% of their current domestic market volume (Destatis 2020). Thus, the use of a single CO_2-source would suffice to provide enough secondary material for consumer products on several different markets.

The results of the CO_2-balances in combination with the economic analysis further reveal an imbalance between benefits and costs of a CO_2-based value chain. The benefits, such as the reduction and the use of secondary carbon and the liquidation of a possible price premium are located at the end of the value chain. At the same time the significant investment requirement in combination with higher production costs than for fossil-based base chemicals illustrate the risks of sunk costs and potential losses at the start. Thus, a successful introduction of a CO_2-based polymer products requires value chain wide cooperation to balance the risks and benefits.

The results of the scenario analysis further show that the future development of factors which indirectly influence the investment costs, such as the plant lifetime also have a decisive impact on the performance of the considered value chains. The declining capex for electrolyzer in combination with increasing plant lifetimes and process efficiencies for the H_2, methanol and monomer production cause a significant decrease in production costs for CO_2-based polymers while the electricity costs hardly change. The oil price development amplifies (increasing price (I)) or counteracts (decreasing price (D)) this trend. An average decrease of the cost difference for the consumer products by 42% (D) to 49% (I) in 2030 and 81 (D) to 85% (I) in 2050 would be achieved. Nevertheless, the production costs remain higher for CO_2-based value chains in all cases since the necessary break-even costs for H_2 between 1.4 – 1.6 (2030) and 2.8 – 3.2 €/kg_{H2} (2050) are not reached. Moreover, the inclusion of CO_2-based polymer production into emission trading schemes would not suffice to enable competitive production costs under status quo conditions or in 2030, independent from the oil price development (Fig. 4). To

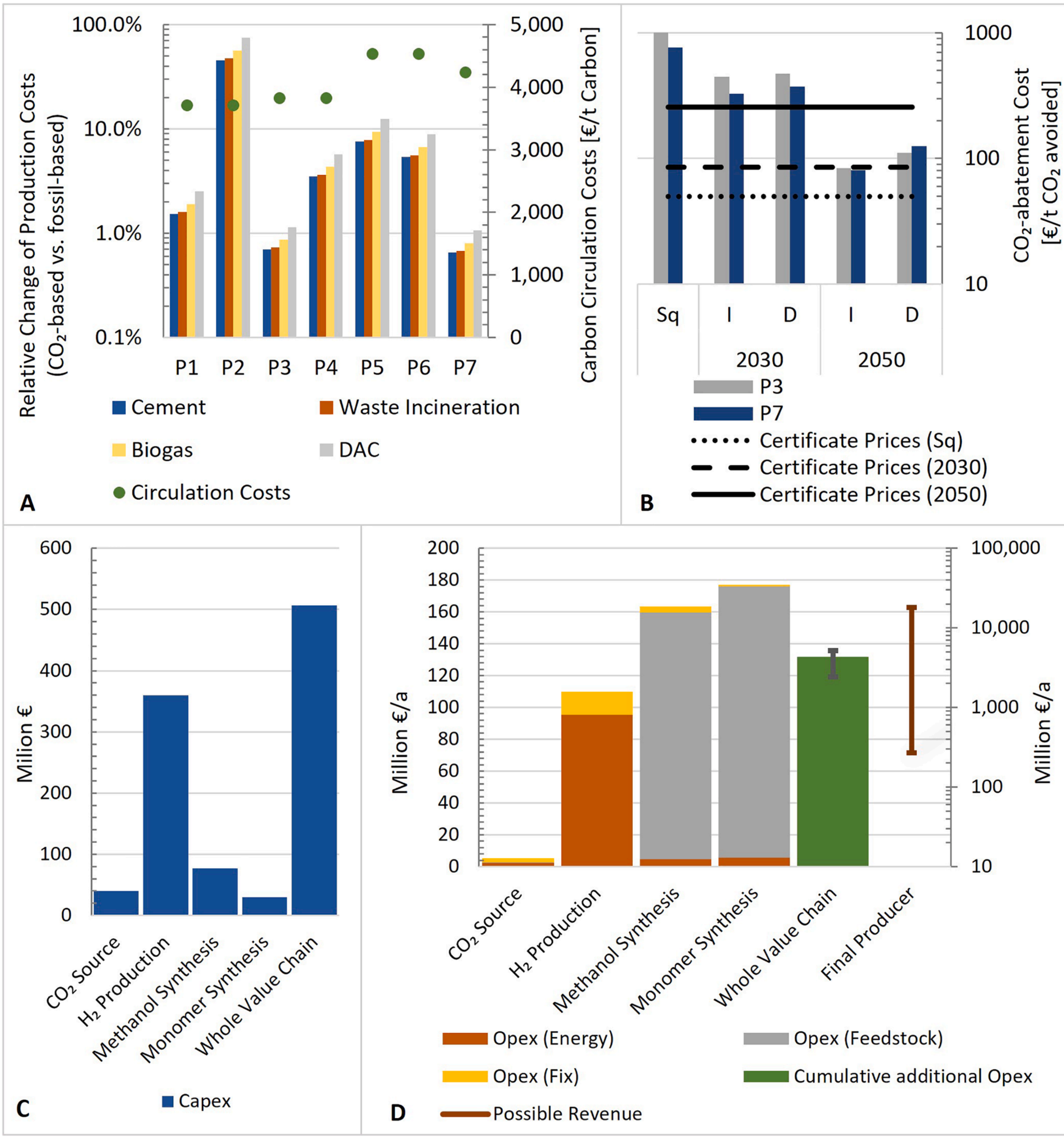

Fig. 4. A) Comparison of the relative change of production costs for CO_2-based polymer products differentiated by the CO_2-source (bars, left y-axis). Comparison of carbon circulation costs for value chains using a cement plant as CO_2-source (right y-axis). **B)** Exemplary development of CO_2-abatement costs for the value chains with a cement plant as CO_2-source which show the highest (P3) and lowest (P7) abatement costs in the Status quo (Sq). For the future scenario, a decreasing (D) and increasing (I) oil price was assumed. The description of the different products can be found in Table 1. **C)** Required new investments (capex) for the different steps of a CO_2-based value chain and the value chain as a whole **D)** Specific Opex for the different steps of CO_2-based ethylene production in combination with the range of the cumulative additional Opex for all regarded CO_2-based value chain options (left y-axis), and the possible revenues for the final product producer (right y-axis). For the CO_2-based value chain a cement plant is considered. As production capacity for CO_2-based feedstock, 100 kt MeOH per year was assumed. (DAC = Direct Air Capture).

reach competitiveness based on avoided emissions, certificate prices greater than 761 (Status quo), 328 (2030) or 57 (2050) €/$t_{CO2,avoided}$ would be necessary. Only in the long-term, this could be an effective option. Break-even oil prices would lie between 199 (POM) – 610 €/Barrel (PP) under status quo conditions, 132 (POM) – 343 €/Barrel (PP) in 2030 and 82 (POM) – 127 €/Barrel (PP) in 2050. Despite the assumed increases in process efficiencies, the CED for CO_2-based processes remains higher (at least 28% in 2050) than for the conventional production, so that CO_2-based value chains will remain more energy intensive in the future.

It must be noted that the values used in this study were derived from the literature and not specifically gathered as primary data. Hence, they involve uncertainties. The sensitivity of the economic results towards certain parameters shows the possible effect of parameter uncertainty as well as future potentials of process improvements. Here, the electricity prices, as well as the efficiencies of the electrolysis and synthesis processes have a high influence on the cost difference to fossil-based alternatives, i.e., the competitiveness of CO_2-based processes. For example, an increase of the efficiency by 1% could lower the additional costs for the CO_2-based alternatives by 0.7% (electrolyzer) or 1.2% (MTO synthesis). At the same time, an increase in electricity costs by the same ratio would raise the cost difference by 0.6%. A corresponding change in plant costs for the electrolyzer, which is the biggest investment position within the value chain, would alter the price difference about 0.4%. Moreover, a deviation of the capital costs for new investments by 1% would change the cost difference by 1.6%. In addition, a raise in market prices for fossil feedstocks would also significantly reduce the cost difference between fossil and CO_2-based products, while the transportation costs and plant costs for CO_2 capture play a minor role. In case of the CO_2 emissions, the carbon intensity of the electricity supply, i.e., scope 2 emissions, is decisive. If the energy system is solely based on renewable energy, carbon neutrality, i.e., net zero emissions, can be reached for CO_2-based polymers, while the emissions of fossil-based polymers would only slightly decrease. The use of the current grid mix instead of wind electricity for the electrolysis step, however, would increase the system wide CO_2 emissions in all cases, instead of decreasing them.

3.3. *Eco-efficiency*

The efficiency scores are used to identify those value chains, i.e., DMUs, which use the available ecological and economic resources in the most efficient way, now and in the future.

Calculating efficiency scores by the mutual comparison of all DMUs yields the following results. First, the share of polymer costs has a significant impact on the eco-efficiency of CO_2-based value chains because it determines the resulting cost difference. For products with a low share of polymer costs, CO_2-based alternatives (P1, P3, P4, P7) show high scores for the eco-efficiency of 1 or close to 1. For products with a higher share of polymer costs (P2, P5, P6), CO_2-based production is comparably inefficient. Thereby, one product made of POM (P7), and one made of PP (P3) are the most eco-efficient CO_2-based value chains (Fig. 5). Second, future reductions in costs and energy requirements would lead to increasing eco-efficiency scores for all CO_2-based alternatives. However, products with a higher share of material costs (P2, P5, P6) remain comparably inefficient. Therefore, certain CO_2-based value chains already represent eco-efficient alternatives to the prevailing fossil-based alternatives, considering the current state of technology. In the future the existing differences for the other CO_2-based value chains are expected to further decrease. Thereby, increasing oil prices would raise the eco-efficiency scores of all CO_2-based value chains. Moreover, the mean deviation of the eco-efficiency score caused by the CO_2-source (10%) is lower than the mean deviation caused by the product type (35%). Thus, the choice of the product has a higher impact on the eco-efficiency than the choice of the CO_2-source. At the same time, CO_2-based value chains using a cement plant as CO_2-source show the highest eco-efficiency score for all products, while using DAC as carbon source represents the most inefficient alternative in all cases. Therefore, the first choices for a CO_2-based value chain should be for products with a low share of polymer costs in combination with a cement plant as CO_2-source, if the described assessment indicators are used.

4. Discussion

This article extends previous studies on the environmental and economic assessment of CO_2-based chemical production by a widened value chain wide perspective. In total, four different CO_2-based value chain setups based on state-of-the-art technologies were compared to the fossil-based alternative for seven different polymer containing consumer products. The value chains were assessed by their economic and environmental performance. The results show that CO_2-based value chains offer environmental advantages while requiring additional energy and higher production costs. For the future, an increase of the environmental benefits can be expected in combination with lower production costs and energy requirements. The results further reveal that the choice of the polymer containing product and the CO_2-source have a decisive impact on the ultimate price premium of the product. For certain consumer products, market readiness of a CO_2-based production and thus an abandonment of fossil carbon could be reached with comparably small price premiums below 1% of the current net market price.

The results of this study extend the existing research in multiple ways. First, previous assessments of carbon recycling technologies, such as Faraca et al. (2019) or Meys et al. (2020) are complemented with an assessment of CCU technologies as carbon recycling pathway. Second, the cash flows of a CO_2-based value chain calculated in this article quantify and confirm the qualitative results by Naims (2020). Based on an extensive literature review, the author showed that the creation of a CO_2-based value chain helps CO_2-emitters by using the otherwise emitted CO_2, offers many investment opportunities for equipment manufacturers (e.g., manufacturers of electrolyzers), and provides improved product characteristics to the producers of consumer products. Building on that, the results of this article enable the organizations involved in CO_2-based value chains to better understand and estimate the possible benefits as well as to calculate the required expenditures.

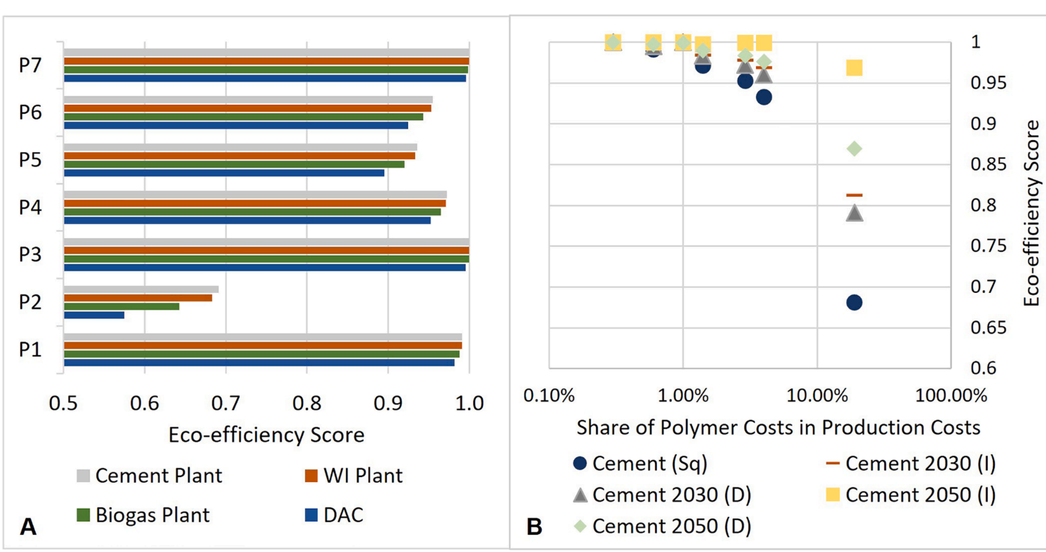

Fig. 5. **A)** Efficiency scores for CO_2-based value chains in the status quo for all case examples (P1 – P7). An efficiency score < 1 means, that there is at least one other value chain which uses the available resources more efficiently. **B)** Relation between efficiency score and the share of polymer costs for the status quo and the scenario, considering a cement plant as CO_2-source. (DAC = Direct Air Capture, WI = Waste Incineration; Sq = Status quo; *I* = increasing Oil prices; *D* = decreasing oil prices).

Not only for the production of chemicals but also for the finally produced consumer products. Third, the impact of the yearly emission volume, i.e., the economies of scale, on the total production costs of chemicals and consumer products was calculated for the first time; this complements the known positive impact of the CO_2-concentration within the feed gas on the possible emission reductions (Hoppe et al., 2017; Müller et al., 2020) as well as economic calculations considering the transport of CO_2 (Zang et al., 2021; Psarras et al., 2017). The current analysis demonstrates the importance to choose the right product and the right CO_2-source to improve the environmental and economic performance of the value chain.

If customers are willing to pay comparably small price premiums, the market potential for CO_2-based polymer products is large. Compared to other sectors where the use of hydrocarbons will most likely continue to play a significant role (e.g., aviation, shipping, or transport on the road) the relative price premiums for the use of CO_2-based hydrocarbons are much higher since the feedstock costs represent a higher share of the total costs. Previous studies showed that a price premium of 32% for commercial flight tickets (Clean Sky 2020), 95% up to 600% for cargo costs via shipping (Lindstad et al., 2015; Stolz et al., 2022) or an increase in the total costs of ownership of 49% for trucks and 165% for passenger cars (Wietschel et al., 2019) would be necessary to enable a cost-covering provision of the same product or service without the use of fossil fuels. The higher value creation of the products analyzed here offers better options to pass the additional costs for feedstocks into the market without causing significantly increased prices for the product or services. Thus, the cost structure of certain polymer products offers an advantage to the chemical and polymer industry in the case of purchasing power for CO_2-based chemicals. Since lower price premiums for sustainable products might lead to a higher willingness to buy sustainable products, the chances to become a successful business model are higher (Eyerund 2015). First collaborations of industrial partners and a supermarket chain are starting to explore this potential by producing CO_2-based bottles for cosmetic products (TotalEnergies 2020) or detergents (MIGROS 2021), which underlines the practical significance of this study's thrust of investigation. In addition, the set-up of regional supply chains using local and unavoidable CO_2-sources creates supply-security.

To further reach competitiveness for CO_2-based value chains on a broad scale and therefore transform them into a successful CEBM, several market entry barriers described by Porter (2014) must be considered. Some of them could be overcome easily. For example, because of the comparably small differences between the production costs, the entry barriers caused by higher costs are nearly negligible for certain products. Moreover, the supply switching transaction costs, i.e., the costs for polymer producers to change their feedstock supply, are comparably low as well. In contrast to mechanical recycling, virgin material without quality degradation or impurities is provided and the existing transport and distribution infrastructure can be used. This makes CO_2-based polymers suitable for application fields with a high demand for product quality and purity, e.g., in the medical or nutrition sector. Here, a thorough comparison between CO_2-utilization and chemical recycling, which could also provide feedstock for high quality polymers, is necessary to identify specific advantages and disadvantages and derive the most suitable application fields for the different carbon recycling technologies.

Other market entry barriers are harder to overcome, and adjustments of the current policies might be helpful to improve the competitiveness of CO_2-based value chains. First, the prevailing fossil industry is established for decades and provides high efficiencies and economies of scale. Second, the build-up of a CO_2-based value chain requires high investment volumes and therefore possible sunk costs, i.e., high investment risks for some of the involved industries (IEA 2018; Gao et al., 2020). Third, the current regulatory policy favors the prevailing fossil production technology by not internalizing the environmental costs into the market. The acceptance of CO_2-based polymers in the proposed recyclate input quotas (European Commission 2020) for polymers could be an important step to incentivize the use of secondary carbon via CO_2-based value chains. In contrast, the inclusion of CO_2-based polymers in emission trading schemes would either have a minor effect or require much higher certificate prices ($>$ 700 €/tCO_2 avoided) than currently the case (50 €/t CO_2 avoided) (World-Bank, 2021). Further measures could also aim at the internalization of environmental costs for fossil fuel use, e.g., through the taxation of fossil fuels used as materials which is already the case for their use as energy carriers.

Based on the results of this study, further research is necessary in several fields. First, a cross comparison with different recycling technologies like mechanical and chemical recycling would help to reveal advantages and disadvantages of the respective technologies in an in-depth manner. It should be examined which technology offers the lowest CO_2-abatement and carbon circulation costs, also considering demands on product quality and purity which has been an issue for mechanical recycling. Second, concrete collaboration strategies and further policy measures should be examined in more detail for all involved industries to level the involved costs and benefits in a fair and competitive way. Third, the combination of non-avoidable CO_2-sources in Germany with imported hydrogen could mitigate the competition for the required renewable energy while creating carbon supply security for the industry. The respective routes for hydrogen supply should be thoroughly assessed.

5. Conclusions

CO_2-based polymer production can become a viable business model for carbon recycling which contributes to the circular economy via closing technical carbon loops. Through a value chain analysis from the CO_2-source until the polymer-based product, promising pathways for the use of CO_2 as carbon source were identified. Even with state-of-the-art technologies and current regulation schemes, the production of products with a high value would require price premiums below 1% compared to the use of fossil polymers. A multi criteria analysis showed that certain CO_2-based products already constitute eco-efficient alternatives to a fossil-based production. For the future, the additional costs can be expected to decrease in combination with increasing process efficiencies which further improves the overall performance of CO_2-based value chains. The investment risks and higher cost at the beginning are faced with possible benefits at the end of the value chain, wherefore costs and benefits are unevenly distributed. This unveils, that cooperation along the value chain is a key aspect to properly level the costs and benefits. Within CO_2-based value chains, economies of scale tend to play an important role, wherefore the choice of the CO_2-source has a significant impact on the resulting performance. Several options exist to accelerate the market introduction of CO_2-based polymer products, e.g., by creating markets for secondary carbon via input quotas. The inclusion into emission trading schemes, however, would not have a decisive impact.

CRediT authorship contribution statement

Simon Kaiser: Conceptualization, Investigation, Methodology, Formal analysis, Data curation, Validation, Writing – original draft, Project administration. **Stefan Gold:** Conceptualization, Methodology, Validation, Writing – review & editing, Supervision. **Stefan Bringezu:** Conceptualization, Validation, Writing – review & editing, Supervision, Funding acquisition.

Declaration of Competing Interest

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

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.resconrec.2022.106422.

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