Climate change mitigation potential of carbon capture and utilization in the chemical industry

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Chemical production is set to become the single largest driver of global oil consumption by 2030. To reduce oil consumption and resulting greenhouse gas (GHG) emissions, carbon dioxide can be captured from stacks or air and utilized as alternative carbon source for chemicals. Here, we show that carbon capture and utilization (CCU) has the technical potential to decouple chemical production from fossil resources, reducing annual GHG emissions by up to 3.5 Gt CO_2-eq in 2030. Exploiting this potential, however, requires more than 18.1 PWh of low-carbon electricity, corresponding to 55% of the projected global electricity production in 2030. Most large-scale CCU technologies are found to be less efficient in reducing GHG emissions per unit low-carbon electricity when benchmarked to power-to-X efficiencies reported for other large-scale applications including electro-mobility (e-mobility) and heat pumps. Once and where these other demands are satisfied, CCU in the chemical industry could efficiently contribute to climate change mitigation.

climate change | carbon capture and utilization | chemicals | renewable energy | circular economy

The chemical industry consumes ∼28% of the industrial and ∼10% of the global final energy (1). Most of this energy is obtained from oil and other fossil resources, which are either used as carbon feedstock (58%) or to generate process energy (42%) (1). While other uses of fossil resources can be directly replaced by renewable energy, the need for a carbon feedstock is expected to make the chemical industry the largest driver for the future increase in global oil demand (2). The chemical industry already reduced the use of fossil resources and the resulting greenhouse gas (GHG) emissions substantially through process intensification and energy efficiency measures, but the potential of these measures has largely been exhausted (3). Consequently, deeper cuts in GHG emissions require more disruptive change such as the use of biomass feedstock (4), electrification (5), carbon capture and storage (6), and carbon capture and utilization (CCU) (3). Here, we analyze the technical potential of CCU to mitigate GHG emissions.

CCU technologies can substitute the conventional production of various chemicals including basic chemicals, fine chemicals, and polymers (7–11). These technologies capture carbon dioxide (CO_2) from industrial point sources or ambient air and use the captured CO_2 as alternative carbon source for chemical production. Replacing conventional chemical production through CCU affects GHG emissions throughout the production chain (i.e., from cradle-to-gate; Fig. 1) by (*i*) removing CO_2 from air or from stacks, (*ii*) avoiding the GHG emissions necessary for conventional chemical production including the supply of raw materials and energy, and (*iii*) adding GHG emissions necessary for CO_2 capture and the conversion of CO_2 into chemicals. Many CCU technologies use hydrogen from electricity-driven water electrolysis to activate the inert CO_2 molecule, offering a route to integrate renewable electricity more significantly into chemical life cycles (12). In contrast, CCU technologies do not affect the use phase and end-of-life (i.e., gate-to-grave) GHG emissions of chemicals if they produce the chemicals with an identical molecular structure as conventional production. In this case, there is no benefit from the temporary storage of carbon within the chemicals during the use phase because the same amount of carbon is stored for the same time (see *SI Appendix* for further discussion).

While climate benefits of some CCU technologies have been reported individually, the global potential of CCU for climate change mitigation is still under debate (13), hampering the integration of CCU into policy frameworks and technology roadmaps (14, 15). Previous estimates (13) of the climate change mitigation potential of CCU relied on the amount of CO_2 stored in products. However, the amount of CO_2 stored can differ substantially from the potential GHG emission reductions due to CCU; using, e.g., 1 kg CO_2 for the production of CO_2-based polymers can reduce up to 3 kg CO_2-eq emissions due to the avoided conventional production (16). Thus, a comprehensive analysis of the climate change mitigation potential of CCU requires a detailed assessment from a life cycle perspective (17, 18).

In this study, we examine the technical potential for climate change mitigation by CCU in the chemical industry. The technical potential is defined here as the maximum GHG emission reductions that are technically feasible through full deployment of CCU technologies (19) with wind power as low-carbon electricity input. We establish a bottom-up model covering the production of 20 large-volume chemicals accounting for over 75% of the chemical industry's GHG emissions (20). Based on this model, we analyze potential disruptive changes through large-scale CO_2 utilization and provide an industry-wide analysis of

Significance

Carbon dioxide (CO_2) drives climate change when released to the atmosphere. Alternatively, CO_2 could be captured and utilized as carbon source for chemicals. Here, we provide a global assessment of the technical climate change mitigation potential of carbon capture and utilization (CCU) in the chemical industry. We develop an engineering-level model of the global chemical industry representing 75% of current greenhouse gas (GHG) emissions. The model allows us to analyze the potential disruptive changes through large-scale CO_2 utilization and resulting emission reductions. Our study shows that CCU has the technical potential to lead to a carbon-neutral chemical industry and decouple chemical production from fossil resources. This transition, however, would cause largely increased mass flows and demand for low-carbon electricity.

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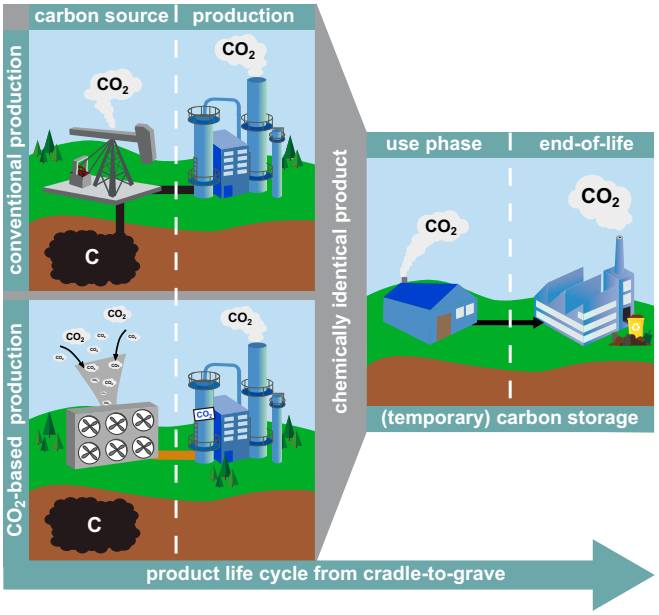


Fig. 1. Changes in the life cycle of established chemicals through the implementation of CCU technologies.

CCU technologies' technical potential to mitigate GHG emissions from a life cycle perspective.

Results

Scenarios for a CCU-Based Chemical Industry. The bottom-up model of the chemical industry yields future production pathways for the production of the 20 large-volume chemicals in 2030 (20) for three scenarios. In the "conventional scenario" (Fig. 2*A*), the chemical industry converts 1.12 Gt of fossil resources into chemicals and generates about 2.0 Gt CO_2-eq cradle-to-gate emissions using conventional production technologies that are already commercialized today. Due to increased demand, this estimate is higher than current GHG emissions of the chemical industry [about 1.5 Gt CO_2-eq in 2013 (19)] and is in line with previous estimates for 2030 (20).

In a second scenario, where the production of the 20 chemicals relies on CO_2-based methanol (21) and methane (22), feedstock mass flows increase substantially by 287% due to the CO_2 used and water coproduced (Fig. 2*B*): 3.72 Gt CO_2 and 0.59 Gt hydrogen from water electrolysis are annually converted into methanol and methane. Methanol is further processed into olefins and BTX, which are the basis of the other large-volume chemicals. Methane substitutes natural gas to produce both heat and ammonia. CO_2 can be captured from two different sources representing the upper and lower bound for the climate impact of CO_2 supply: a highly concentrated industrial point source (~100% CO_2) and ambient air with about 400 ppm CO_2 (23). This scenario leads basically to the methanol economy envisioned by Asinger (24) and promoted by Olah (25). Since all technologies in this scenario are at technology readiness levels (TRLs) of 7 and higher, this scenario is denoted "high-TRL scenario." The integration of CO_2 via methane and methanol would require comparably low research and development efforts and allows use of wide parts of the existing petrochemical infrastructure and technologies.

The third scenario further includes CCU technologies for the direct conversion of CO_2 into olefins (26, 27), BTX (28), carbon monoxide (3), ethylene oxide (29), and styrene (30) (*SI Appendix*, Fig. S1). These technologies are currently at early research and development stages with TRLs below 7. Therefore, this scenario is denoted "low-TRL scenario." The direct synthesis of chemicals from CO_2 reduces the amount of CO_2 and hydrogen needed to 2.77 and 0.38 Gt, respectively, but mass flows are still about 182% larger compared with the conventional scenario. Due to the early development stages of these technologies, the realization of this scenario would require substantial research and development efforts and novel production facilities. Since this scenario is based on low-TRL technologies, all calculations are subject to increased data uncertainty. The employed methodology to estimate life cycle assessment (LCA) results for low-TRL technologies is presented in *SI Appendix*.

In the CCU scenarios, hydrogen produced via water electrolysis represents the major source of energy for the chemical industry. Electricity demands amount to about 32.0 PWh in the high-TRL scenario and 18.1 PWh in the low-TRL scenario. Electricity demands could be reduced through direct use of hydrogen from water electrolysis. For example, the direct use of hydrogen in ammonia production could reduce the electricity demand in the low-TRL scenario by 7.5% by avoiding the steps for methanation and steam reforming in the production of ammonia from CO_2-based methane (details in *SI Appendix*). However, these production pathways are not based on CO_2 and therefore excluded from the CCU scenarios. For the CCU scenarios, the electricity demands in the high- and low-TRL scenario correspond to about 97% and 55% of the expected world electricity production in 2030 according to the new policy scenario of the International Energy Agency (IEA) (31), respectively. Hence, CCU in the chemical industry could only reduce GHG emissions on the large scale with the joint massive expansion of electricity production capacities. As a result, the carbon footprint of electricity from the technologies used to expand the electricity production capacities will determine the climate benefits of CCU.

Climate Change Mitigation Depending on Electricity Supply. We found that the GHG emission reductions of replacing conventional chemical production through CCU varies widely depending on the carbon footprint of electricity (Fig. 3). Our results show that CCU can substantially reduce GHG emissions in both CCU scenarios, but only if low-carbon electricity is available. In the high-TRL scenario, CCU technologies reduce life cycle GHG emissions compared with conventional technologies once the employed electricity has a carbon footprint of 260 g CO_2-eq/kWh or lower. The life cycle GHG emissions of the chemical industry decline nonlinearly as function of the carbon footprint of electricity since our optimization approach minimizes GHG emissions and different CCU technologies start to outcompete the corresponding conventional technologies in terms of their life cycle GHG emissions at different carbon footprints of electricity. Electricity carbon footprints where CCU technologies enter the production mix in the model range from 74 g CO_2-eq/kWh (mixed xylene) to 260 g CO_2-eq/kWh (methanol; *SI Appendix*, Table S1). For all technologies, capturing CO_2 from the industrial point source leads to higher emission reductions than air capture, because less energy is required for capture (23). GHG emissions are most reduced by using CO_2 from the industrial point source and electricity from wind power, because wind power is currently the energy generation technology with the lowest carbon footprint. The resulting maximum GHG emission reduction is the difference between the GHG emissions of the conventional and of the CCU scenario. The life cycles of conventional and CCU technologies differ only from cradle-to-gate, while emissions during the use phase and end of life, as well as potential benefits from carbon storage are identical in all scenarios since the same chemicals are produced. The maximum GHG emission reductions amount to 3.4 Gt CO_2-eq per year and represent the technical GHG mitigation potential of the scenario. Emissions are reduced by replacing emission-intensive processes within the chemical industry and its supply chain, and by capturing

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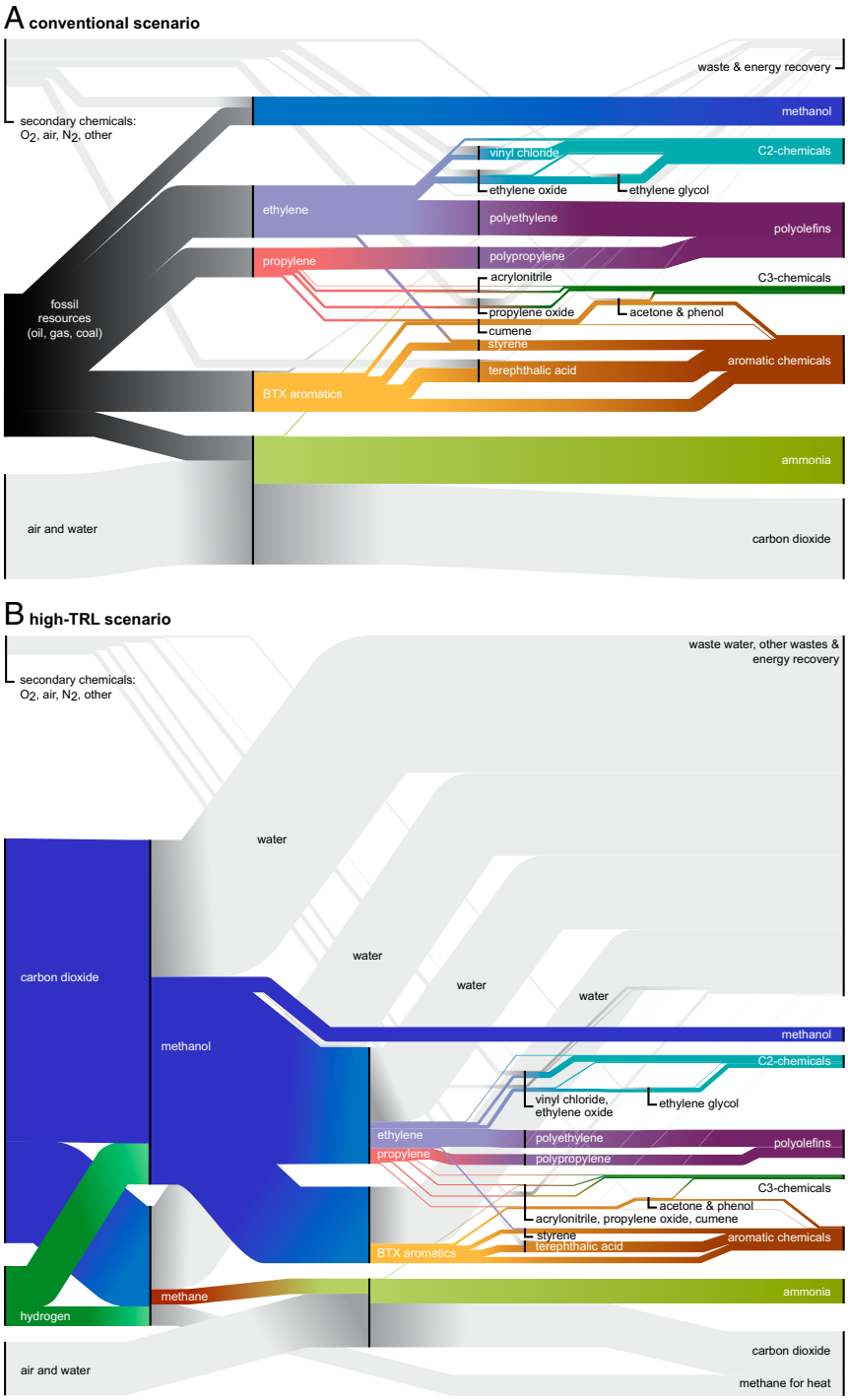


Fig. 2. Mass flows within the chemical industry in (*A*) the conventional scenario and (*B*) the high-TRL scenario for CCU implementation. In both scenarios, the projected final demand for 20 large-volume chemicals in 2030 is produced. Note, mass flows are scaled differently in the conventional and the high-TRL scenario. The mass flows of the final demand (on the *Right*) are identical.

CO_2 outside the boundaries of the chemical industry. The resulting structure of the chemical industry is presented in Fig. 2*B*.

In the low-TRL scenario, moderate climate impact reductions are achieved regardless of the carbon footprint of electricity, because this scenario also includes CCU technologies that do not require electricity for hydrogen production, i.e., synthesis of ethylene from CO_2 and methane, and ethylene oxide from CO_2 and ethylene. However, also in the low-TRL scenario, emissions can be substantially reduced only with low-carbon electricity. CCU technologies become beneficial for electricity carbon footprints between 44 g CO_2-eq/kWh (carbon monoxide) and 334 g CO_2-eq/kWh (paraxylene; *SI Appendix*, Table S1). In the low-TRL scenario, the annual emissions are reduced from 4.2 Gt CO_2-eq for the conventional scenario to 0.7 Gt CO_2-eq leading to a maximum climate change mitigation potential of 3.5 Gt CO_2-eq per year.

To contextualize the required carbon footprints of electricity, we show the current carbon footprint of grid electricity for different

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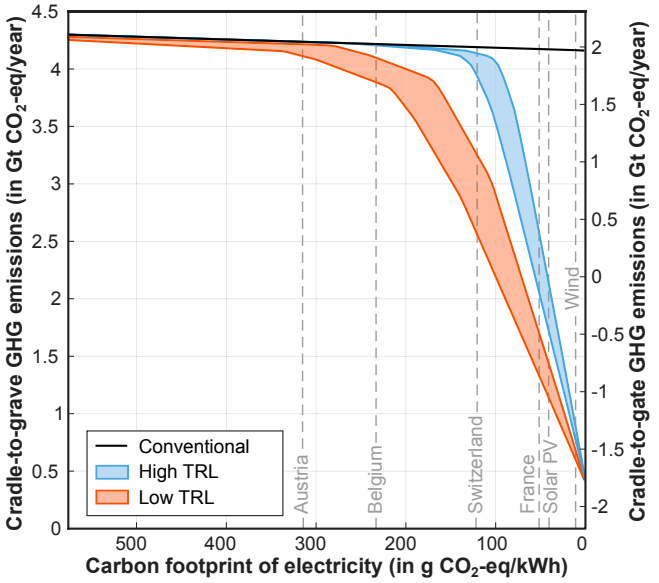


Fig. 3. Cradle-to-grave and cradle-to-gate GHG emissions of the chemical industry producing the final demand for 20 large-volume chemicals in 2030 as function of the carbon footprint of electricity. Cradle-to-grave emissions include all emissions throughout the life cycles of the 20 large-volume chemicals, while cradle-to-gate emissions cover only the production stage and the supply of all raw materials and energy needed for production. The vertical dashed lines illustrate the climate impact of grid electricity in selected countries or of electricity from selected renewable energy technologies.

countries and technologies in Fig. 3. While most countries and technologies do not provide electricity with a sufficiently low carbon footprint to realize substantial GHG emission reductions by CCU, there are countries where CCU could reduce GHG emissions substantially using grid electricity already today. In France, for example, the introduction of high-TRL CCU technologies would roughly halve the climate impact of chemicals over the entire life cycle.

Even though individual countries have already demonstrated that low-carbon electricity can be provided at scale, the transformation of the chemical industry toward CCU would cause a substantial demand for additional electricity that would require a large-scale expansion of electricity production capacities. This expansion would require large shares of renewable (or nuclear) energy to achieve a sufficiently low carbon footprint.

If all additional electricity were provided by renewable energy, the amount of renewable energy required for the full-scale introduction of CCU would correspond to 126% and 222% of current targets [sustainable development scenario of IEA (31)] for the global renewable electricity production in 2030 for the low-TRL and the high-TRL scenario, respectively. Even these current targets are already known not to be achievable based on existing and announced policies (31). Thus, the need for a further expansion of renewable electricity production capacities is likely to be a limiting factor for CCU in the chemical industry.

The climate change mitigation potential of CCU technologies depends on both the amount of additional electricity available and the carbon footprint of electricity (Fig. 4). The amount of additional electricity available determines the scale of CCU implementation and resulting GHG emission reductions. For a given electricity carbon footprint, the climate impact of the chemical industry depends nonlinearly on the amount of electricity available, because individual CCU technologies differ in their efficiencies in using renewable energy to achieve emission reductions. Our model allocates additional electricity to the CCU technologies that save the largest amount of GHG emissions until the demands for the chemicals from such technologies are exhausted (*Materials and Methods*). Additional electricity is thus progressively allocated to CCU technologies reducing GHG emissions less efficiently. As a result, the slope of the GHG emissions decreases with the amount of additional electricity available. For carbon-free electricity, efficiencies of CCU technologies range from 340 g CO_2-eq avoided per kilowatt hour for the production of paraxylene to 140 g CO_2-eq avoided per kilowatt hour for the production of methane. Hence, higher emission reductions per kilowatt hour can be achieved, if the limited low-carbon electricity is used for the most efficient CCU technologies.

Discussion

Considering both the large potential of CCU in the chemical industry to mitigate climate change and the large amount of low-carbon electricity needed to exploit this potential, we should ask ourselves two questions: (*i*) Can we provide that much low-carbon electricity, and, if yes, (*ii*) should we use it in the chemical industry?

According to a recent Intergovernmental Panel on Climate Change (IPCC) report (32), the amount of renewable energy that could be produced by full implementation of demonstrated technologies exceeds even the most ambitious scenarios for renewable energy deployment in 2050 by more than one order of magnitude. Thus, in theory, it is possible to produce sufficient low-carbon electricity. However, the actual implementation of renewable energy capacities is limited by practical constraints including costs, competition for land, public acceptance of energy infrastructure, and limits in the uptake of intermittent electricity supply by the electricity grid (33). Despite the remarkable

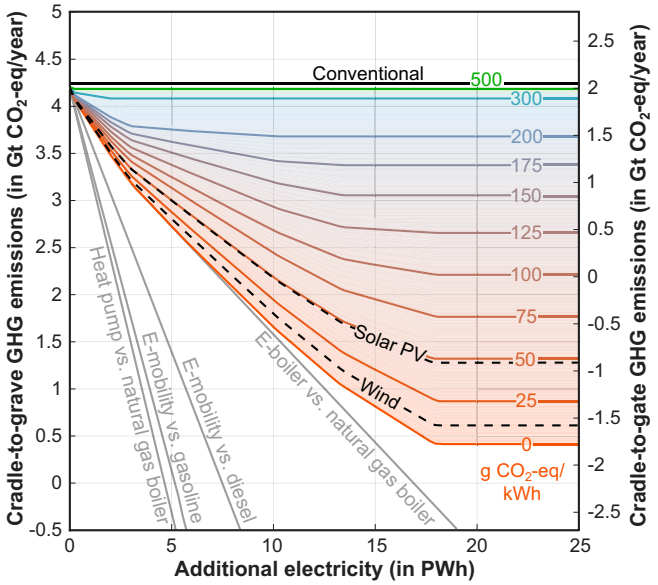


Fig. 4. Cradle-to-grave and cradle-to-gate GHG emissions for the chemical industry in the low-TRL scenario producing the final demand for 20 large-volume chemicals in 2030 as function of the amount of additional electricity available and its carbon footprint in grams of CO_2 equivalent/kilowatt hour. Cradle-to-grave emissions include all emissions throughout the life cycles of the 20 large-volume chemicals, while cradle-to-gate emissions cover only the production stage and the supply of all raw materials and energy needed for production. The black solid line represents the GHG emissions in the conventional scenario. The light gray lines illustrate potential GHG emission reductions by using the additional electricity for e-mobility to substitute gasoline or diesel cars, or for heat generation in a heat pump or an e-boiler to substitute heat from natural gas boilers.

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technological progresses and substantial reduction in cost, modern nonhydro renewable power, including wind, solar, biomass, geothermal, and ocean power, accounts for only 1.7% of the global final energy demand (34). Hence, dramatically increasing low-carbon electricity to the extent that it can sufficiently power CCU for chemicals in the next decade is likely to be a challenge, and renewable energy is expected to remain a limited resource for the coming decades.

In this case, how much of the limited, low-carbon electricity resource should be allocated to CCU technologies compared with other potential uses for low-carbon electricity? For this question, it is useful to differentiate between on- and off-grid use of renewable electricity. For on-grid use, the additional low-carbon electricity for CCU is distributed via the electricity grid. In this case, the electricity could also be used by other GHG mitigation technologies connected to the grid such as electromobility (e-mobility) or heat pumps. From the point of climate change mitigation, limited low-carbon electricity should be used for those technologies that reduce the climate impact the most (5, 35). In Fig. 4, as an example, we show the climate impact reduction by substituting natural gas boilers with either heat pumps or electric boilers, as well as substituting diesel or gasoline cars through e-mobility. Power-to-heat and power-to-e-mobility are both very large-scale uses of renewable electricity and would thus compete with CCU for electricity. The climate impact reductions have been calculated based on power-to-X efficiencies by Sternberg and Bardow (5) for the use of emission-free electricity from surplus power. The power-to-X efficiency represents the climate impact reductions per electricity used (details in *Materials and Methods*). In comparison with all hydrogen-based CCU technologies considered in this work, e-mobility and heat pumps reduce the climate impact more strongly per kilowatt hour of electricity used. Hence, from a climate perspective, the implementation of these technologies should be prioritized over the hydrogen-based CCU technologies considered in this work until their demand for renewable energy is fully exhausted. However, hydrogen-based CCU implementation in the chemical industry still provides a later option for climate change mitigation, since large-scale emission reductions will eventually be needed in all relevant sectors (19). Similarly, even the installation of electric boilers to substitute natural gas boilers reduces the climate impact more than all hydrogen-based CCU technologies except the CO_2-based production of para-xylene and styrene. Still, climate benefits are achieved by CCU technologies that do not require electricity for hydrogen production such as the production of ethylene and ethylene oxide.

However, the perspective changes in remote areas without grid connection but with large unused renewable energy resources. Here, off-grid CCU technologies could provide climate benefits without competing with other technologies for renewable energy. Even more, by transforming regionally bound renewable energy into transportable commodities, CCU technologies could enable global trade of renewable energy, for example, in the form of CO_2-based methanol or methane. Also, ammonia could be used as renewable fuel (36, 37). However, ammonia is produced more efficiently by the direct conversion of renewable hydrogen with nitrogen than by CCU (*SI Appendix*). Setting up production plants in remote areas will result in additional costs for infrastructure, feedstock supply (e.g., CO_2 and water), and the transportation of the CO_2-based product (e.g., methanol) to established chemical production sites for further processing. For the CO_2-based production of methanol in remote areas, for example, additional transportation costs for the CO_2 supply from industrial point sources and the transportation of methanol have been estimated to about 100 USD/t, i.e., about 25% of current methanol production costs based on fossil resources (37). These additional costs, however, will partly be offset by lower renewable electricity prices and higher load factors in the world's most favorable production regions (37). Using hourly wind and solar geospatial data, Fasihi et al. (38) identified wide areas, where a combination of one-axis sun-tracking solar photovoltaic capacities and modern wind turbines could enable water electrolysis with load factors higher than 50%. Many of these areas are located in Africa, Australia, and South America, where the amount of available renewable energy resources is more than 50 times higher than the current total primary energy demand (32). Even though our study does not quantify potential climate benefits from using CO_2-based energy vectors outside the chemical industry, the trade of renewable energy through CO_2-based products could be highly beneficial especially for densely populated regions such as Germany, Japan, or Korea that have fewer renewable energy resources and may in practice fall short of employing sufficient capacities to satisfy their future renewable energy demand (32).

The presented analysis focuses on the technical potential for climate change mitigation by CCU in the chemical industry in 2030, i.e., the maximum reduction of climate impacts that is technically feasible in case of full deployment of CCU (Fig. 2). The actual deployment rate, however, is likely to be lower. First, achieving full deployment of novel CCU technologies by 2030 would imply an average annual increase in market penetration of 10% between 2020 and 2030. This increase in market penetration substantially exceeds current replacement rates of chemical production plants: Assuming an average plant life time of 25 y (39), only 4% of existing production capacities are replaced annually. Consequently, even though parts of the existing chemical infrastructure could still be used, a rapid implementation of CCU technologies would require substantially higher investment volumes, as well as the phase out of existing production plants before the end of their technically feasible lifetime. Second, the full implementation of CCU technologies can only be achieved with a massive expansion of low-carbon electricity production capacities that substantially exceeds current targets for low-carbon electricity production for 2030 (31). This expansion is likely to represent a bottleneck for large-scale hydrogen-based CCU implementation within the next decades. Furthermore, the expansion will be based on a mix of electricity generation technologies leading to a higher carbon footprint than wind power assumed for the technical potential in this study. Third, in addition to CCU, other measures have been proposed for reducing climate impacts in the chemical industry including the use of biomass feedstock (4), electrification (5), and carbon capture and storage (6). Thus, climate impacts of the chemical industry are likely to be reduced by a mix of measures.

The technical climate change mitigation potential of CCU is affected by the CO_2 source. Capturing CO_2 from highly concentrated CO_2 sources such as industrial point sources reduces emissions more, because less energy is required for capture than for dilute sources such as air. The emissions reductions capture how much emissions are changing as consequence of introducing CCU technologies. However, for the goal of an overall zero-emission society, the industrial point source itself would have to be de-fossilized or end-of-life emissions from the CCU product would need to be avoided, e.g., by permanent carbon storage. In contrast, direct air capture and biogenic point sources (e.g., biobased ethylene production) would allow for a closed carbon cycle even if the CCU product is incinerated. Switching toward lower concentrated sources will increase costs due to higher energy demands for CO_2 capture. In a net-zero emission economy, CCU could then provide the carbon feedstock needed for the production of a wide range of products (e.g., chemicals, plastics, and pharmaceuticals).

While a detailed economic assessment of CCU in the chemical industry is currently not possible due to the early development stage of most CCU technologies, the magnitude of additional operational cost can be estimated based on major cost factors

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Table 1. Technologies for CCU implementation in the high- and low-TRL scenario

Chemical	High-TRL scenario	Low-TRL scenario
Benzene	Methanol-to-aromatics (42)	$9\ CO_2 + 27\ H_2 \rightarrow C_6H_6 + 18\ H_2O + 3\ CH_4$ (28)
Carbon dioxide	Capture from highly concentrated point source or ambient air (23)	Capture from highly concentrated point source or ambient air (23)
Carbon monoxide		$CO_2 + H_2 \rightarrow CO + H_2O$ (3, 49)
Ethylene	Methanol-to-olefins (42)	$2\ CO_2 + 2\ CH_4 \rightarrow C_2H_4 + 2\ CO + 2\ H_2O$ (26) $2\ CO_2 + 6\ H_2 \rightarrow C_2H_4 + 4\ H_2O$ (27, 54)
Ethylene oxide		$C_2H_4 + CO_2 \rightarrow C_2H_4O + CO$ (29)
Hydrogen	From water electrolysis (50)	From water electrolysis (50)
Methane	From CO_2 (Sabatier reaction) (51, 52)	From CO_2 (Sabatier reaction) (51, 52)
Methanol	From CO_2 and H_2 (direct hydrogenation) (53)	From CO_2 and H_2 (direct hydrogenation) (53)
Propylene	Methanol-to-olefins (42)	$3\ CO_2 + 9\ H_2 \rightarrow C_3H_6 + 6\ H_2O$ (27, 54)
Styrene		$C_8H_{10} + CO_2 \rightarrow C_8H_8 + CO + H_2O$ (30)
Toluene	Methanol-to-aromatics (55)	$9\ CO_2 + 26\ H_2 \rightarrow C_7H_8 + 18\ H_2O + 2\ CH_4$ (28)
Xylene, mixed	Methanol-to-aromatics (55)	$9\ CO_2 + 25\ H_2 \rightarrow C_8H_{10} + 18\ H_2O + CH_4$ (28)
Xylene, para	Methanol-to-aromatics (55)	$9\ CO_2 + 25\ H_2 \rightarrow C_8H_{10} + 18\ H_2O + CH_4$ (28)

Low-TRL technologies are represented by the chemical equations of the underlying reactions.

including the avoided annual consumption of crude oil (4.21 billion barrel) and natural gas (6.59 PWh) and the production of hydrogen from low-carbon electricity in the CCU scenarios (0.38 Gt and 0.59 Gt in the low- and high-TRL scenario). With expected prices in 2030 of 92.3 USD per barrel oil [current policy scenario (31)], 0.017 USD per kWh natural gas (40), and 1.8–3.5 USD per kg hydrogen (41) from renewable energy in most beneficial production regions (lower limit) and regions with good but not excellent solar and wind resources (upper limit; Europe or similar), the additional operating cost for the full implementation of CCU technologies in the low- and high-TRL scenario amount to 185–833 and 564–1,570 billion USD annually, respectively. These additional costs correspond to 19–87% and 59–164% of the market value of the produced chemicals according to 2017 prices (42). The corresponding climate change mitigation costs range between 52–235 USD per t CO_2-eq and 168–467 USD per t CO_2-eq in the low- and high-TRL scenario. For the low-TRL scenario, the lower bound of the climate change mitigation costs from this simplified calculation are thus in the range of expected carbon prices for the year 2030 (19). This estimate, however, neglects all required investment cost within the chemical industry except for hydrogen production by water electrolysis. In the CCU scenarios, investment costs are likely to increase, because larger mass flows need to be moved: The mass flow of hydrogen and CO_2 needed is 1.8 and 2.9 times larger than the mass flow of fossil inputs in the low- and high-TRL scenario, respectively. The larger mass flows will lead to larger production facilities. The increase in investment costs will add to the CO_2 mitigation costs of CCU.

Previous studies have discussed the potential role of CCU for climate change mitigation based on the amount of CO_2 utilized (15, 43). The High Level Group of Scientific Advisors to the European Commission, for example, recently reported an estimated long-term utilization potential of 1–2 Gt per year (15). Alternatively, the amount of CO_2 stored in chemicals has been used as simplified indicator for the climate change mitigation potential of CCU (13). In contrast, the modeling approach proposed in this study provides a detailed assessment of GHG emission reductions due to disruptive changes through large-scale CCU implementation. The lack of models for assessing disruptive changes has recently been identified as priority research need for LCA of CCU (44). Our results show that the climate change mitigation potential of CCU in the chemical industry is neither determined by the amount of CO_2 used, nor stored in chemicals, but by the substitution of conventional technologies. Therefore, estimates based on the amount of carbon used or stored should be interpreted with caution. GHG emission reductions due to substitution have been demonstrated for individual CCU technologies (3), but not for a large-scale CCU implementation in the global chemical industry. Finally, our analysis highlights the need to determine not only emission reductions compared with conventional technologies, but to also compare climate change mitigation measures regarding their power-to-X efficiency.

The presented analysis focuses on the climate change mitigation potential of CCU and neglects CCU services beyond climate change mitigation (35). For example, CO_2-based fuels could reduce the import dependency of countries that do not produce fossil fuels by enabling a diversification of energy supply, and hence increase energy security. Furthermore, CCU products can reduce other environmental impacts, e.g., NOx and particular matter emissions from fuels (45). Such benefits need to be considered to comprehensively assess the potential of CCU. For climate change mitigation, our results provide a basis for the sound integration of CCU into research agendas, technology roadmaps, and future policy frameworks.

Materials and Methods

Scope of the Model and Key Assumptions. The bottom-up model of the chemistry industry yields future production pathways for 20 major bulk chemicals: acrylonitrile, ammonia, benzene, caprolactam, cumene, ethylene, ethylene glycol, ethylene oxide, methanol, mixed xylenes, phenol, polyethylene, polypropylene, propylene, propylene oxide, p-xylene, styrene, terephthalic acid, toluene, and vinyl chloride. Production pathways are represented by more than 160 processes based on engineering-level data. Thereby, flows of energy and materials are determined in detail throughout entire supply chains. The key assumptions of the model are illustrated below, while the computational structure is shown in the following section.

Technology choices. Technologies are chosen to minimize GHG emissions, enabling the determination of the theoretical maximum climate change mitigation potential by CCU compared with a non-CCU scenario. For each chemical, both conventional and CO_2-based production technologies are considered. For the conventional production pathways, only the best-available technologies (BATs) from a climate perspective are included, i.e., the industrialized technologies with the lowest climate impact per kilogram product. The focus on BATs implies a conservative estimate of the climate change mitigation potential of CCU technologies.

CO_2 supply. For the CO_2 supply, we consider two potential sources representing the upper and lower bound for the climate impact of CO_2 supply: a highly concentrated industrial point source (~100% CO_2) and ambient air with about 400 ppm CO_2 (23).

Use phase and end of life. Emissions during the use phase are neglected. As end-of-life scenario, we assume the incineration of all chemicals in a waste incinerator, leading to 2.2 Gt CO_2-eq emissions. The assumption of waste incineration is a worst-case assumption for end-of-life emissions. Assuming waste incineration neglects that parts of the chemicals may also be stored in

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Table 2. Key assumptions and parameters of the calculations of the power-to-X efficiencies of e-mobility and power-to-heat by Sternberg and Bardow (5)

E-mobility	Value	Ref.
Battery electric vehicle with lithium ion battery		
Battery efficiency	80%	
Electricity consumption of battery electric vehicle	0.14–0.2 kWh·km^{-1}	56, 57
Fuel consumption of gasoline car	0.52 kWh·km^{-1}	58
Fuel consumption of diesel car	0.38 kWh·km^{-1}	58
Power-to-heat		
Electricity consumption of heat pump	2.1–4.9 kWh·kWh$_{heat}^{-1}$	59
Electricity consumption of electric boiler	1 kWh·kWh$_{heat}^{-1}$	
Natural gas demand of natural gas boiler	1.1 kWh·kWh$_{heat}^{-1}$	58

materials for substantially long times. Also, the waste incineration plant could add facilities for CO_2 capture and sequestration. However, both the use phase and the end of life of chemicals are assumed to be identical, because all CCU technologies considered produce the identical chemicals as conventional production. Therefore, potential benefits from temporary carbon storage or sequestration will be the same in the conventional and the CCU scenarios, and not affect the difference in GHG emissions, i.e., the climate change mitigation potential.

CCU scenarios. The CCU scenarios include all technologies from the conventional scenario and technologies for CCU implementation. The technologies for CCU implementation are illustrated in Table 1. The methodology for data collection and a list of all processes and data sources is provided in *SI Appendix*. In all scenarios, processes for the disposal of wastes and for energy integration and recovery are included.

Computational Structure of the Bottom-Up Model. The bottom-up model of the chemical industry builds on the technology choice model (TCM) (46). Following the general definitions of LCA (47), the technical production system is described by four basic entities: technologies, intermediate flows, elementary flows, and the final demand. Technologies are defined as activities transforming inputs into outputs. Input and output flows of energy, materials, or products are categorized into intermediate flows and elementary flows. Intermediate flows are flows between technologies, such as intermediate products or raw materials. Elementary flows are exchanged between technologies and the environment, such as emissions of GHGs or resources extracted from the environment. The output of products for final consumption is specified by the final demand.

The data on the physical production system are structured according to the generalized calculus for LCA (47). The transformation of intermediate flows by technologies is described by the technology matrix A. In this matrix A, columns represent production technologies, while rows indicate intermediate flows. A coefficient a_{ij} of the technology matrix A shows the intermediate flow i that is produced (for $a_{ij} > 0$) or consumed (for $a_{ij} < 0$) by technology j. Analogously, the consumption and emission of elementary flows by technologies is represented by the elementary flow matrix B. In this matrix, a coefficient b_{ej} describes the elementary flow e that enters (for $b_{ej} < 0$) or leaves (for $b_{ej} > 0$) technology j. The final demand is represented by the final demand vector y, where an element y_i describes the final demand for intermediate flow i.

For the production of various chemicals in the model, more than one production technology is included. Choices between technologies are determined by the minimization of the climate impact of the entire production system. To quantify the climate impact, a scaling vector s is defined, which scales the amount of inputs and outputs of each technology, thus describing the production level. Based on this scaling vector, the cumulated elementary flows g of the production system that are exchanged with the environment throughout the entire life cycle of chemicals are determined by the following:

$$g = Bs. \quad [1]$$

Following leading guidelines for life cycle impact assessment (48), these cumulated elementary flows g are further characterized regarding their contribution to climate change using the characterization vector Q. An element q_e of Q represents the 100-y global warming potential of elementary flow e according to IPCC (19), illustrating the relative contribution of this flow to climate change over a 100-y time horizon. By this means, the climate impact can be expressed as CO_2-equivalents of GHG emissions according to the following equation:

$$h = QBs. \quad [2]$$

Based on these definitions, the linear program of the bottom-up model of the chemical industry is defined by the following equations (Eqs. **3**–**6**):

$$Min\ h = QBs, \quad [3]$$

$$s.t.\ As = y, \quad [4]$$

$$s \le c, \quad [5]$$

$$s_j \ge 0, \quad [6]$$

where h represents the climate impact of the production system, A specifies the technology matrix, y is the final demand, and c is potential upper bounds for scaling vector entries. An upper bound has been set for the amount of electricity available in the calculations for Fig. 4. Eq. **3** expresses the climate impact minimization objective under the constraints that the final demand is produced (Eq. **4**) and that the scaling vector entries are between zero and the upper bound (Eqs. **5** and **6**).

Determination of Power-to-X Efficiencies of E-Mobility and Power-to-Heat. The climate impact reductions for the benchmark power-to-X technologies are determined based on power-to-X efficiencies by Sternberg and Bardow (5). The power-to-X efficiencies are defined as climate impact reductions per megawatt hour of electricity used and represent the slopes of the gray lines in Fig. 4. In Sternberg and Bardow (34), the power-to-X efficiencies $GW_{reduction}$ are determined based on the following equation:

$$GW_{reduction} = M_{product}\ GW_{conv} - GW_{ESS}. \quad [7]$$

The power-to-X technology uses 1 MWh of electricity to produce the amount $M_{product}$ of its product. Thereby, the conventional production of this amount of product is avoided, reducing global warming impacts by ($M_{product}$ GW_{conv}), where GW_{conv} is the global warming impact of conventional production of one product unit. GW_{ESS} represents the global warming impact of the power-to-X technology using 1 MWh of electricity. For both power-to-X and substituted technologies, emissions due to operation and construction are considered. Key assumptions and parameters of the calculations of the power-to-X efficiencies of e-mobility and power-to-heat are illustrated in Table 2.

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