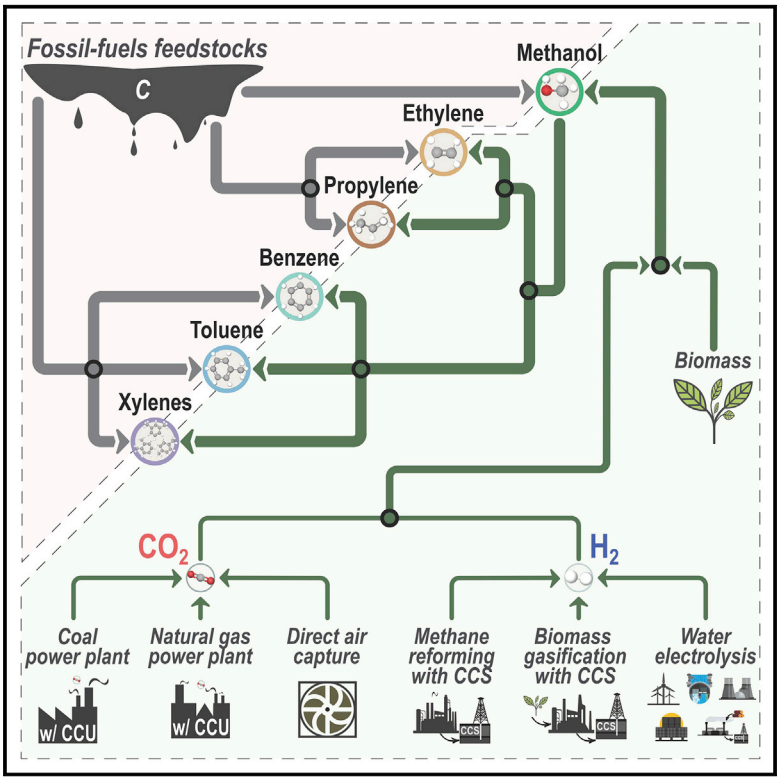
Article

One Earth

Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries

Graphical abstract



Highlights

- The petrochemical industry requires 25% of Earth's operating capacity
- Sustainability of 50 "renewable" carbon routes for the petrochemical sector was examined
- Routes with largest CO_2 savings transgress Earth's biodiversity boundary by 30%
- Planetary boundaries should be incorporated in decarbonization planning

Authors

Ángel Galán-Martín, Victor Tulus, Ismael Díaz, Carlos Pozo, Javier Pérez-Ramírez, Gonzalo Guillén-Gosálbez

Correspondence

jpr@chem.ethz.ch (J.P.-R.), gonzalo.guillen.gosalbez@chem.ethz.ch (G.G.-G.)

In brief

Transformative actions to decarbonize the chemical sector, such as using alternative non-fossil carbon feedstocks, should be assessed relative to the planetary boundaries to understand the overall environmental implications. Our study reveals that replacing fossil feedstocks with "renewable" carbon can reduce CO_2 emissions by 25% to 100%. However, the technology pathways that offer the highest CO_2 mitigation could compromise biosphere integrity. Our work highlights the importance to consider overall sustainability in decarbonizing hard-to-abate sectors.

Galán-Martín et al., 2021, One Earth *4*, 565–583
April 23, 2021
https://doi.org/10.1016/j.oneear.2021.04.001

CellPress

One Earth

Gold Standard for the Global Goals | 3 tons of CO_2 offset

CellPress OPEN ACCESS

Article

Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries

Ángel Galán-Martín,[1,5] Victor Tulus,[1,2,5] Ismael Díaz,[3] Carlos Pozo,[4] Javier Pérez-Ramírez,[1,*] and Gonzalo Guillén-Gosálbez[1,6,*]

[1]Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1, 8093 Zürich, Switzerland

[2]Departament d'Enginyeria Química, Universitat Rovira i Virgili, Av. Països Catalans 26, 43007 Tarragona, Spain

[3]Departamento de Ingeniería Química Industrial y del Medio Ambiente, ETSI Industriales, Universidad Politécnica de Madrid, C/ José Gutiérrez Abascal 2, 28006 Madrid, Spain

[4]LEPAMAP research group, University of Girona, C/ Maria Aurèlia Capmany 61, 17003 Girona, Spain

[5]These authors contributed equally

[6]Lead Contact

*Correspondence: jpr@chem.ethz.ch (J.P.-R.), gonzalo.guillen.gosalbez@chem.ethz.ch (G.G.-G.)

https://doi.org/10.1016/j.oneear.2021.04.001

SCIENCE FOR SOCIETY Using novel decarbonization technologies to curb carbon emissions in the hard-to-abate industrial sectors has received increasing attention in combatting climate change. However, sustainability assessments of such technologies are often limited to carbon footprint analyses and CO_2-emission-saving potential.

Here, we assessed the impact of transitioning away from fossil and toward renewable carbon feedstocks in the petrochemical industry relative to Earth's nine planetary boundaries. We found that decision- and policy-making focused solely on mitigating CO_2 emissions in the petrochemical sector could lead to actions that severely exacerbate biodiversity loss and compromise Earth's resilience. Our results highlight the need for holistic environmental analyses beyond carbon mitigation potential to guide low-carbon transitions underpinning sustainable development.

SUMMARY

The petrochemical sector will play a crucial role in developing low-carbon transition technologies, but the industry also contributes a significant proportion of greenhouse gas emissions. Momentum is building to help reduce the carbon footprint of this hard-to-abate sector, particularly through replacing fossil carbon feedstocks with carbon from biomass, captured CO_2, and other recycled resources, but the broader implications of these so-called "solutions" remain unclear. Here, we assess the overall sustainability of such "renewable carbon pathways" by quantifying their life-cycle environmental footprints with respect to the previously defined nine planetary boundaries. We show that although a shift toward renewable carbon pathways could indeed reduce CO_2 emissions by 25% to over 100%, the scenario with the lowest carbon footprint could exceed the biodiversity planetary boundary by at least 30%. Our work highlights the potential pitfalls of overlooking global environmental guardrails beyond greenhouse gas emissions reduction and identifies new avenues for quantifying the environmental footprint of decarbonization solutions for hard-to-abate sectors.

INTRODUCTION

The chemical industry is what is known as a hard-to-abate sector. This sector has a significant carbon footprint, but it is also important in providing everyday materials and developing low-carbon technologies to aid a transition to a stable and sustainable future.[1] It is estimated that the sector contributes 1.24 Gt CO_2-eq annually, accounting for about 10% of global total final energy consumption and 7% of greenhouse gas (GHG) emissions associated with industry.[2] The primary source of emissions within the sector is energy use obtained primarily from fossil resources; other sources include those associated with chemical processes

and indirect emissions. Because a large majority of the emissions are associated with the production of chemicals based on carbon feedstocks, electrifying the energy source or deploying carbon capture and storage (CCS) would not fully prevent the sector's strong reliance on fossil carbon as a feedstock.[3] Hence, shifting to feedstocks from renewable carbon—i.e., carbon obtained from captured CO_2, biomass, or recycling chemicals—has become an appealing strategy to help curb the chemical sector's emissions, contribute to the Paris climate targets,[4–7] and, arguably, improve the sustainability of chemical products.[7–9] Here, we refer to such an approach as using "renewable carbon" rather than the conventional "fossil carbon."

The chemical industry is particularly problematic, because the already large demand for chemicals and associated products is expected to further increase sharply.[2] Notably, petrochemicals dominate the feedstock aspect of the chemical industry as a whole, meaning a focus on reducing their environmental footprint is particularly necessary. The main building blocks of the petrochemical industry, which act as precursors to several fine and bulk chemical products, include the following platform chemicals: ethylene, propylene, benzene, toluene, xylenes, and methanol (Figure 1). Ammonia is also an incredibly important platform chemical, but it is not considered here because it does not contain carbon. These platform chemicals, which consume around one-third of the total energy demand of the sector[2] are also currently produced from fossil carbon (i.e., oil, coal, and natural gas) via cracking of naphtha, ethane, and/or liquefied petroleum gas (LPG).

In recent years, a great deal of research has arisen regarding green or low-carbon approaches to chemical manufacture. The aforementioned six platform chemicals could, for example, be generated via the said renewable carbon approaches, either directly or through using so-called "green" methanol as an intermediate to olefins and aromatics, i.e., via methanol-to-olefins (MTO) and methanol-to-aromatics (MTA) processes. The intermediate green methanol itself could be directly produced from renewable biomass resources or by the hydrogenation of captured CO_2. In the case of the latter, H_2 can be generated from biomass or water (with the vast amounts of energy supplied by renewable power sources, e.g., wind, solar, bioenergy with CCS [BECCS][5,10,11]), and the required CO_2 could be captured either at point sources or directly from the air (via direct air capture [DAC]) and then converted into economically valuable chemicals via various technologies.[12,13] Collectively, these approaches are generally referred to as carbon capture and utilization (CCU) and arguably offer a route toward a closed-carbon chemical sector[14–16] or even deliver a negative emissions balance by permanently storing CO_2 in specific plastics or construction materials.[8] Furthermore, different types of biomass resources—including energy crops and residues—could be used to provide biogenic carbon feedstock for chemical conversion following the biorefinery concept,[17] which can also potentially achieve carbon neutrality by consuming naturally captured CO_2.

The transition to a chemical industry based entirely on renewable carbon clearly offers a number of new, exciting, and in some cases economically beneficial opportunities to decrease the environmental impacts of the chemical sector and potentially co-benefits beyond emissions reduction.[1,18–20]

However, such a transition also poses significant challenges. Despite growing interest in emerging technologies based on renewable carbon, their global environmental implications remain largely unexplored due to the narrow scope of current environmental assessments. Notably, most environmental studies often evaluate single technologies focusing on carbon emissions and global warming (GW) and fail to consider the impact on other aspects of the environment. For example, Pérez-Fortes et al.[21] analyzed the net CO_2 used in green methanol from CO_2 and electrolytic H_2, whereas Sternberg et al.[22] quantified the carbon footprint of several CO_2-based C1 chemicals. However, the exhaustive review from Cuéllar-Franca and Azapagic[12] already highlighted the need to consider a wider range of life-cycle assessment (LCA) impacts in CCU to avoid focusing on GW only.

There are only a few studies that have sought to take a more holistic approach to analyze the impact of CCU in the chemical sector. Otto et al.[15] quantified the large-scale CO_2 avoidance potential of 123 CO_2-based routes, considering their production volume in the 27 European Union states, and used it together with other selection criteria to identify the most promising pathways. Mac Dowell et al.[23] quantified the present and short-term global uses of CO_2 by considering 11 different routes, concluding that CCU alone could not cope with the global mitigation challenge. Similarly, Kätelhön et al.[5] quantified the total climate change mitigation potential of CCU in the chemical industry, concluding that it could decouple chemical production from fossil resources while curbing annual GHG emissions by up to 3.5 Gt CO_2-eq in 2030. However, each of these studies only focuses on carbon-emissions reduction potential, which has, up until now, been considered the primary environmental threat; hence, they overlook other relevant impacts that could worsen when attempting to combat climate change.

That is not to say some studies have not looked beyond climate change impacts. Meunier et al.,[24] for example, analyzed a range of environmental impacts in CCU (i.e., methanol production) and identified trade-offs between carbon footprint and water and metal/mineral depletion. Recently, Thonemann[25] conducted a meta-analysis of 52 peer-reviewed articles that deal with LCA and CO_2-based chemical production and evaluated the impact of production in relation with 15 impact indicators, concluding that no one technology performs better across said categories in comparison with conventional production. Similarly, Gabrielli et al.[7] discussed, but only qualitatively, trade-offs between the carbon footprint and the use of resources (land, material and minerals, fossil carbon, and water) in three technology chains that would enable a carbon-neutral chemical industry (i.e., carbon capture and storage coupled with the current infrastructure, as well as two CCU routes), highlighting that there is no clear winner among them. Finally, in a recent study, green methanol production was evaluated related to its impact on eight planetary boundaries, but, again, this is limited in scope.[11] Hence, a holistic assessment quantifying how the large-scale deployment of CCU can affect the stability of Earth is, therefore, still needed.

The planetary boundaries (PBs) concept provides a more holistic and robust framework to evaluate impacts on climate change and beyond in decision-making for global sustainability.[26] The PBs define a set of critical biophysical limits on key

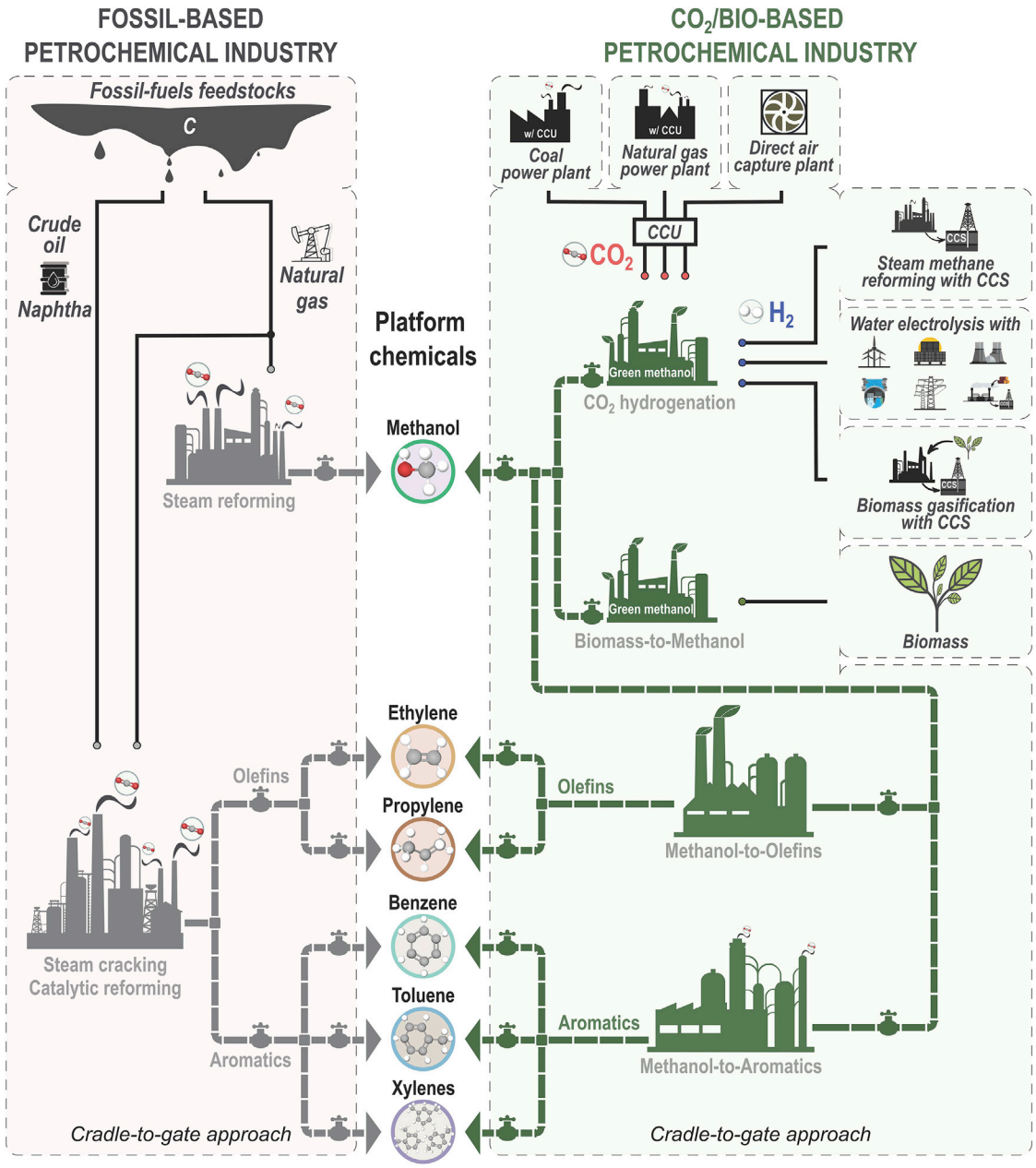


Figure 1. Conceptual framework for replacing the current fossil-based petrochemical industry by its CO_2-based/bio-based analog relying on "green" methanol as intermediate

51 scenarios are considered: (i) fossil-based petrochemical industry, i.e., *Fossil* scenario (on the left), which represents the conventional production of platform chemicals from fossil resources; and (ii) 50 potential alternative scenarios based on *CCU* and biomass resources (on the right), which produce platform chemicals from green methanol synthesized directly from biomass or via CO_2 hydrogenation. Cradle-to-gate system boundaries are considered under the assumption that the downstream routes from platform chemicals to other chemicals are the same across scenarios, and the same applies to the end-use phases of such chemicals.

Earth-system processes whose transgression could potentially shift the current state of the planet.[27,28] Quantitative thresholds for nine Earth-system processes were identified that jointly define a safe operating space (SOS) for maximum anthropogenic perturbation, i.e., an environmental budget to be shared among all anthropogenic activities; in this context, any PBs' transgression could seriously compromise our well-being.[28–32]

Here we introduce a bottom-up approach that quantifies the life-cycle environmental impacts of a renewable-carbon transition of the chemical sector, for the six aforementioned platform chemicals, through the lens of Earth's PBs (Figure 1). Our approach combines a PB characterization framework[33] with an ecological footprint method developed by Hanafiah et al.[34] Our method calculates a "holistic" sustainability indicator, i.e., the PB footprint,

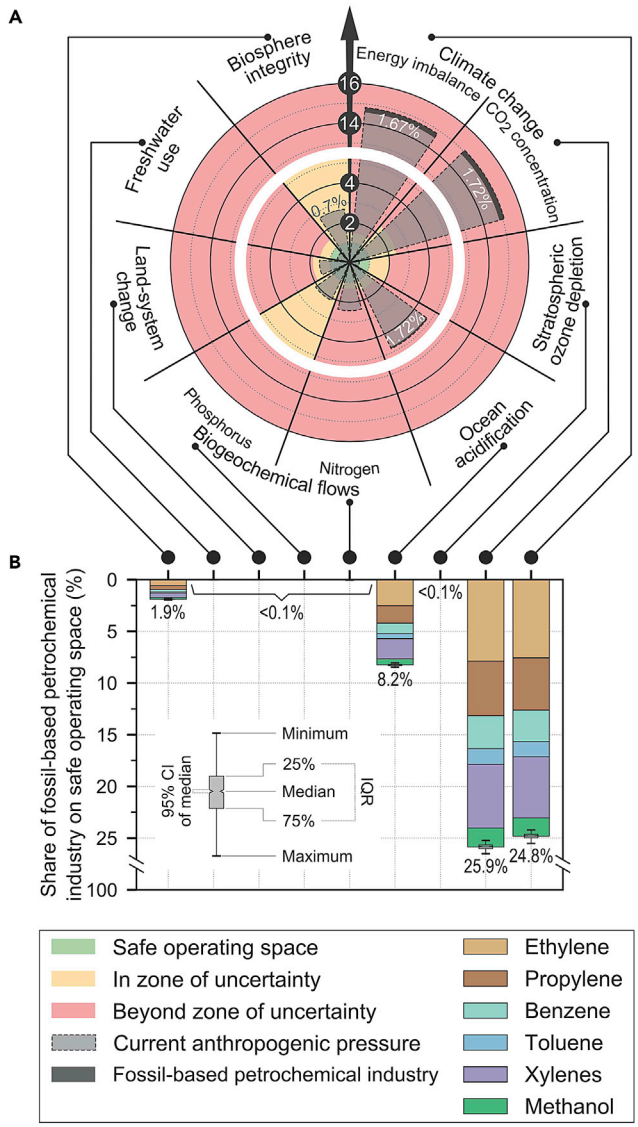


Figure 2. Performance of the fossil-based chemical industry satisfying the demand of platform chemicals in 2020

(A) The current global anthropogenic status of the control variables for the nine PBs, where the axis corresponds to the transgression level, i.e., relative performance with respect to the SOS (SOS = 1). The green zone depicts the SOS, the yellow zone corresponds to the zone of uncertainty, and the red zone is the risk zone. The gray region shows the current level of impact of all the anthropogenic activities, where the part in black corresponds to the share of the fossil-based chemical industry. The current anthropogenic pressures exerted on the climate change, ocean acidification, and biosphere integrity Earth-system processes were adjusted considering current emissions levels and the latest available estimates of the biodiversity intactness index (experimental procedures).

(B) The share of the SOS occupied by the fossil-based chemicals for each PB. Boxplots over the bars indicate the variation in performance considering the uncertainty associated with the inventory data with whiskers excluding outliers according to the 1.5 interquartile rule (experimental procedures).

which offers an advance beyond conventional LCA studies (see experimental procedures).[35] Our analysis compares a *Fossil* scenario (the current petrochemical industry's approach of converting fossil resources into chemicals), taken as a baseline, with 50 alternative renewable carbon scenarios that each rely on green methanol as intermediate (details of all scenarios and how they differ are presented in Note S1 with the schematic representation shown in Figure S1, and modeling calculations and uncertainty analysis are shown in the experimental procedures).

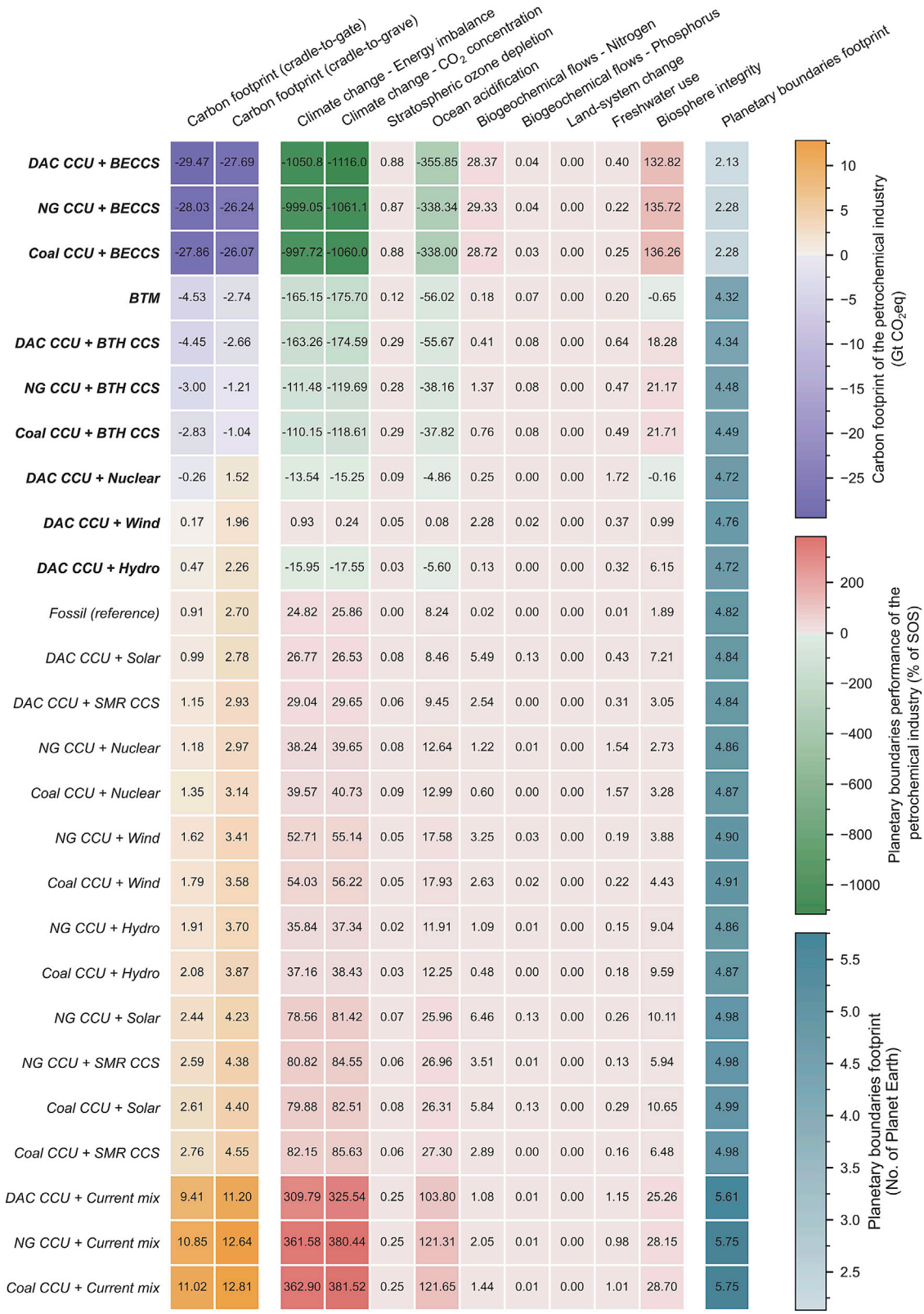
We find that under current practices, the carbon emissions of the fossil-based chemical industry require one-quarter of the entire operating capacity of the planet , which, as expected, raises serious concerns about its sustainability. We show that shifting to a chemical industry entirely based on renewable carbon could alleviate the current PB footprint, but there are a number of potential trade-offs, particularly critical in some biomass routes. Notably, scenarios allowing for the highest levels of carbon-emissions reduction—which are based on bioenergy with carbon capture and storage—exceed the biodiversity PB threshold by 30%, primarily through land-use requirements. A portfolio of renewable-carbon approaches has potential to achieve a transition within PBs, but competition with other sectors for energy resources and economic and sociopolitical barriers could hamper this transition.

RESULTS

Impacts of the fossil-based petrochemical industry

We start by analyzing the *Fossil* scenario based on the current fossil platform chemicals with a total forecasted annual demand of 613.6 Mt for 2020.[2] Here, methanol is produced from natural gas, whereas ethylene, propylene, benzene, toluene, and xylenes, building blocks representing the backbone of the chemical industry, are generated via steam cracking of naphtha from crude oil distillation (Figure 1). Despite currently consuming 24% of the total fossil fuel feedstock input to the chemical industry,[36] ammonia production is omitted because it does not contain carbon. The six platform chemicals are responsible for 0.91 Gt CO_2-eq $year^{-1}$ (over the life cycle), i.e., 46% of the total annual carbon dioxide emissions embodied in the top 20 (on a volume basis) chemicals in 2030 (2.0 Gt CO_2-eq $year^{-1}$).[2,5] In global terms, the GHG emissions attributed to the six platform chemicals represent almost 2% of the annual 52 Gt CO_2-eq linked to anthropogenic activities,[1] a relatively low share (in comparison with other sectors, e.g., transport and power generation) that fails to highlight the need to defossilize this industry.

A different picture emerges when quantifying the PBs' performance relative to the SOS as the global budget to operate sustainably, particularly considering that some PBs have been already crossed as result of human impacts (Figure 2A). Notably, in climate change energy imbalance, climate change CO_2 atmospheric concentration, and ocean acidification, all of them strongly connected to GHG emissions, the same platform chemicals represent 24.82%, 25.86%, and 8.24%, respectively, of the maximum allowable impact at the global Earth-system level (Figure 2B). They are followed by biosphere integrity (1.89%) and then by negligible contributions in the other PBs (<0.02%), all of them more strongly linked to other anthropogenic activities, mainly agriculture.[32] The fossil-based petrochemical industry, therefore, already requires one-quarter of the entire carrying capacity of the planet to operate. This large share far exceeds the contribution of the chemical sector to the world's gross domestic



(legend on next page)

product , i.e., 7.1% in 2017,[37] raising concerns about the fairness of its current impact level in a sustainable economy. In the end, the equitable distribution of the SOS is an open discussion, but the political decisions should consider different perspectives on distributive fairness.[38]

Analyzing the contribution of the fossil-carbon-intensive chemical industry to the current global PB transgression levels, we find that its full replacement, assuming an analog with zero impact, would improve the carbon-related Earth-system processes more substantially. Notably, this replacement would lead to 1.67% reductions in the current transgression level in energy imbalance (from 14.82 to 14.57 times the SOS), 1.72% in CO_2 concentration (from 15.07 to 14.81 times the SOS), and 1.72% in ocean acidification (from 4.80 to 4.72 times the SOS), followed by biosphere integrity (0.70%, from 2.68 to 2.66 times the SOS) (Figure 2A). In contrast, replacing the current fossil-carbon-intensive chemicals would not significantly affect the remaining Earth systems, i.e., changes below 0.01% in the current global performance.

The breakdown of impacts shows that ethylene, propylene, and xylenes altogether account for more than two-thirds of the total impact in the two climate change PBs and in ocean acidification, i.e., 30%, 20%, and 23%, respectively, whereas the contribution of methanol is less significant, i.e., 7% (Figure 2B). This is due not only to the higher demand for olefins and aromatics but also to their higher impact on these PBs per kilogram of chemical compared to methanol (Figures S2–S7; Note S1); this high impact is, in turn, tightly connected to their carbon footprint.[39] Notably, methanol is obtained from a lighter feedstock (natural gas), whereas the other chemicals are produced from the heavier naphtha (and also ethane, in the case of ethylene, or LPG in the case of olefins and aromatics), which leads to larger carbon footprints.

Decarbonizing the energy inputs consumed by the chemical industry would indirectly reduce the impact of the *Fossil* scenario. However, these improvements would be insufficient to make the standard fossil industry sustainable, because its fossil carbon would accumulate in the atmosphere after the use phase of chemicals. Capturing this carbon in the end-use phase of the chemical products would not be a sustainable option either, because this would require unlimited storage capacity for the industry to operate sustainably for many decades to come.

Our results, therefore, highlight the urgent need to make hydrocarbon-based platform chemicals more sustainable, particularly concerning their impact on the climate change PBs already surpassed globally as a result of anthropogenic activities, and where they show the most significant contributions to the SOS. Moreover, the expected three-fold increase in the demand for chemicals by 2050[2] makes the need to defossilize chemicals even more pressing.

Environmental impacts of shifting to renewable carbon

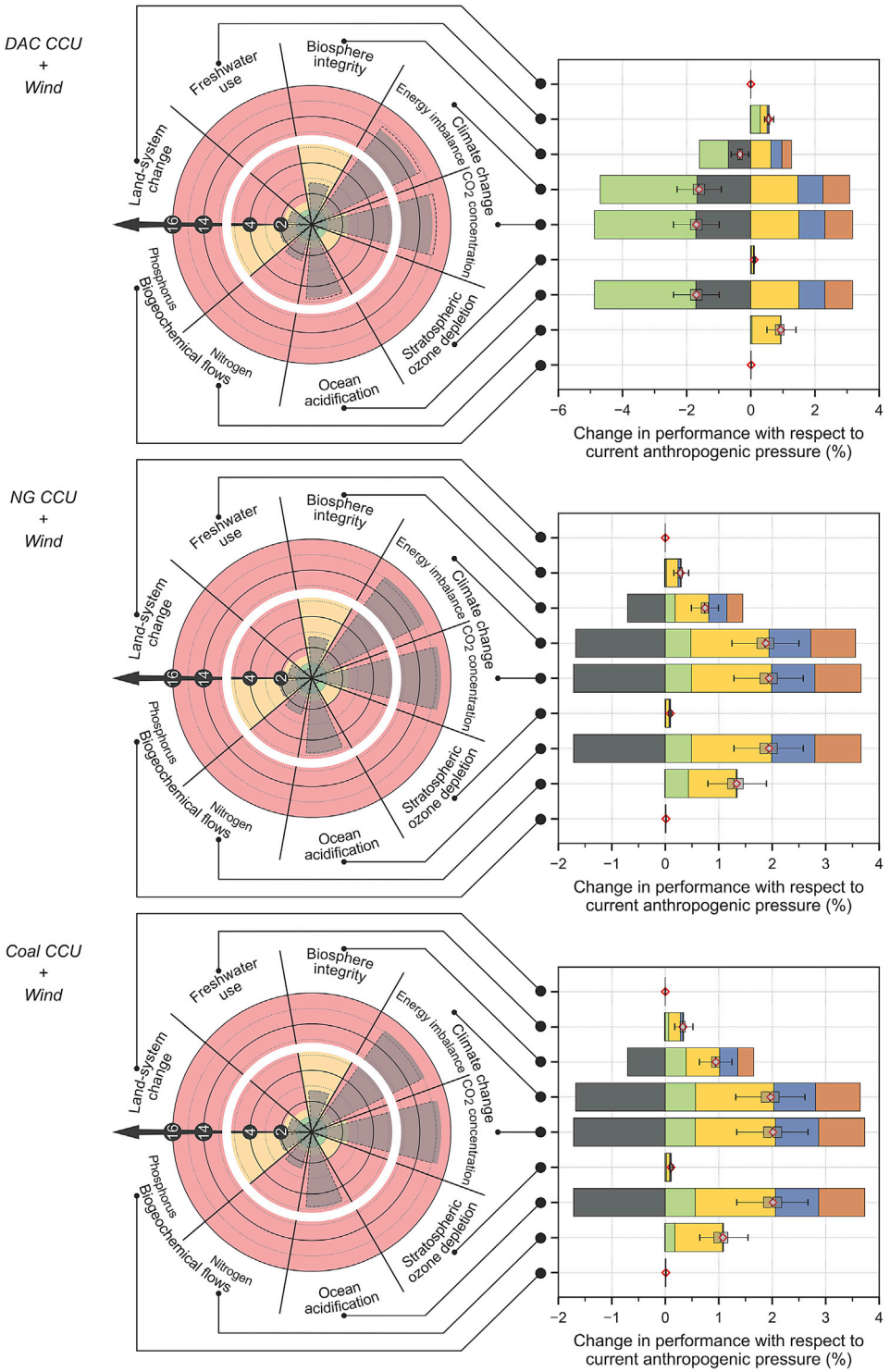
We next study the environmental implications of replacing the petrochemical industry with an analog based on renewable carbon by considering 50 alternative scenarios relying on green methanol. Methanol is first produced, either via hydrogenation of CO_2 or directly from biomass, and subsequently converted into the six platform chemicals through the MTO and MTA technologies. All the scenarios assume that the downstream synthesis routes converting such platform chemicals, traditionally produced from fossil carbon (i.e., naphtha or ethane/LPG), into several products would remain unaltered. Other dedicated direct routes from biomass or CO_2 to chemicals (not relying on methanol as intermediate) might be superior environmentally and economically. However, herein we focus on MTO and MTA because of their high technology readiness levels (TRLs) and the fact that they would imply minimum changes in current infrastructure.[4,5]

We first apply the standard-carbon footprint-based analysis to the scenarios based on the current power mix (Figure 3; equivalent results for a future mix based on prospects are presented in Figure S8 and discussed in Note S2). We find that shifting to scenarios relying on biogenic carbon or CO_2 captured from the air (except for the scenarios relying on H_2 from steam methane reforming [SMR] with CCS or electrolytic H_2 powered by solar or the current mix) would substantially reduce the carbon footprint of the chemical industry in comparison with the footprint produced by current practices (from 0.91 Gt CO_2-eq $year^{-1}$ in the *Fossil* scenario to negative emissions standing at −29.47 Gt CO_2-eq $year^{-1}$ in the *DAC CCU + BECCS* alternative). Among those based on CO_2 captured from natural gas or coal plants, only the ones relying on H_2 from biomass (*BTH CCS*) or electrolytic H_2 from BECCS would reduce the carbon footprint relative to the *Fossil* case.

The largest reductions would correspond to captured CO_2 from air combined with electrolytic H_2 powered by BECCS (*DAC CCU + BECCS*), followed by the biomass-to-methanol (*BTM*) scenario, CO_2 from DAC with H_2 produced via gasification of biomass with CCS (*DACC CCU + BTH CCS*), and then the DAC scenarios relying on nuclear, wind, and hydro followed by the *Fossil* scenario itself. Overall, the DAC scenarios would perform better than those relying on CO_2 from natural gas (*NG CCU*), followed by CO_2 from coal (*Coal CCU*), mainly because the CO_2 from the air was modeled as a negative-emission entry in contrast to the CO_2 captured from power plants (details in the experimental procedures). Notably, the *NG CCU + BECCS* and *Coal CCU + BECCS* scenarios (top three in Figure 3) would also provide substantial carbon-footprint savings due to the massive amount of carbon-negative electricity from BECCS required for the electrolytic H_2. However, these scenarios should be deemed unsustainable because they rely on fossil CO_2, which might prologue the reliance on fossil fuels. Moreover, extra savings of −1.44 Gt CO_2-eq $year^{-1}$ would be achieved by using CO_2 capture from the atmosphere (*DAC CCU + BECCS*), which represents almost double the responsibility of the current petrochemical industry (i.e., 0.91 Gt CO_2-eq $year^{-1}$ in *Fossil* scenario). Furthermore, only those scenarios combining biomass with CCS

Figure 3. Carbon footprint, share of the global SOS occupied by the chemical industry, and PB footprint for each scenario considering the current electricity mix

Rows in the heatmap correspond to the scenarios ranked according to their carbon footprint. Each set of metrics uses a different color key according to the bar legends on the right where corresponding units are indicated. Acronyms and descriptions for the scenarios can be found in Note S1; those labeled in bold show lower carbon and PB footprint than in the *Fossil* scenario. See also Figure S8.



(legend on next page)

(permanent storage of the CO_2), i.e., electricity from BECCS or H_2 from BTH CCS, would lead to net-carbon-negative emissions on a cradle-to-grave basis (assuming the full incineration/degradation of the chemicals, which would result in additional emissions of 1.79 Gt CO_2-eq $year^{-1}$). We note that the *BTM* scenario should be carbon neutral at most (on a cradle-to-grave basis), because the biogenic carbon used as feedstock would be eventually released back to the atmosphere. In practice, however, it also leads to negative carbon emissions due to the omission of the carbon footprint of its by-products (e.g., methane). Overall, focusing solely on the carbon footprint, the *DAC CCS + BECCS* would emerge as superior given its outstanding performance in terms of carbon emissions, i.e., −29.47 versus 0.91 Gt CO_2-eq $year^{-1}$ in the *Fossil* scenario.

We next analyze the same scenarios through the lens of PBs to study their broad environmental implications at the global Earth-system level (Figure 3 for the current mix; results for the future mix in Figure S8). To this end, we apply our bottom-up PB-LCA method to simulate the consequences at the planet level of replacing the fossil-based chemical industry with each alternative scenario. Our method, which avoids downscaling (i.e., assigning budgets of the SOS to a given system, a methodological step on which there is no scientific consensus yet), provides an absolute sustainability index, i.e., the PB footprint, that facilitates the analysis. We define the PB footprint as the average global transgression level of the PBs that would result from substituting the current fossil scenario with an alternative one, assuming that all the other activities in the economy remained the same, i.e., *ceteris paribus* conditions (all other conditions remaining equal). Lower *ceteris paribus* transgression levels would therefore imply lower PB footprints and better absolute environmental sustainability performance in the scenario assessed.

In practice, staying within PBs should be the result of a collective effort among countries and sectors. Hence, alternatives that improve the overall performance but are hard to combine with other strategies that aim at meeting all the PBs concurrently should be discarded. Accordingly, solutions taking a large share of the global SOS in at least one Earth system should be ruled out, because they would leave little room for the other sectors to operate within PBs. As an example, a scenario reducing the global transgression level substantially but consuming the full environmental budget available in at least one Earth system should be deemed unsustainable. Based on these observations, our PB-LCA method analyzes both the global performance in terms of the PBs (i.e., PB footprint) and the individual impact on each Earth system (i.e., share of the SOS occupied in each Earth system).

In essence, the aggregated metric leads to the same ranking of alternatives (results shown in blue in Figure 3), with only ten scenarios reducing the PB footprint compared with the *Fossil* scenario (labeled in bold in Figure 3). Moving toward a future mix based on the Sustainable Development Scenario of the World Energy Outlook[40] would reduce the impact in all the PBs, resulting in 12 scenarios improving the *Fossil* scenario (the same as with the current mix, plus the *DAC CCU + SMR CCS* and *DAC CCU + Solar* scenarios, Figure S8). Similarly, as in the carbon-footprint analysis, the *DAC CCU + BECCS* scenario yields the lowest PB footprint (i.e., 2.13) (Figure 3). This is because the scenarios with lower GHG emissions entail more significant reductions in climate change and ocean acidification Earth-system processes, which show at present the largest global transgression levels (Figure 2).

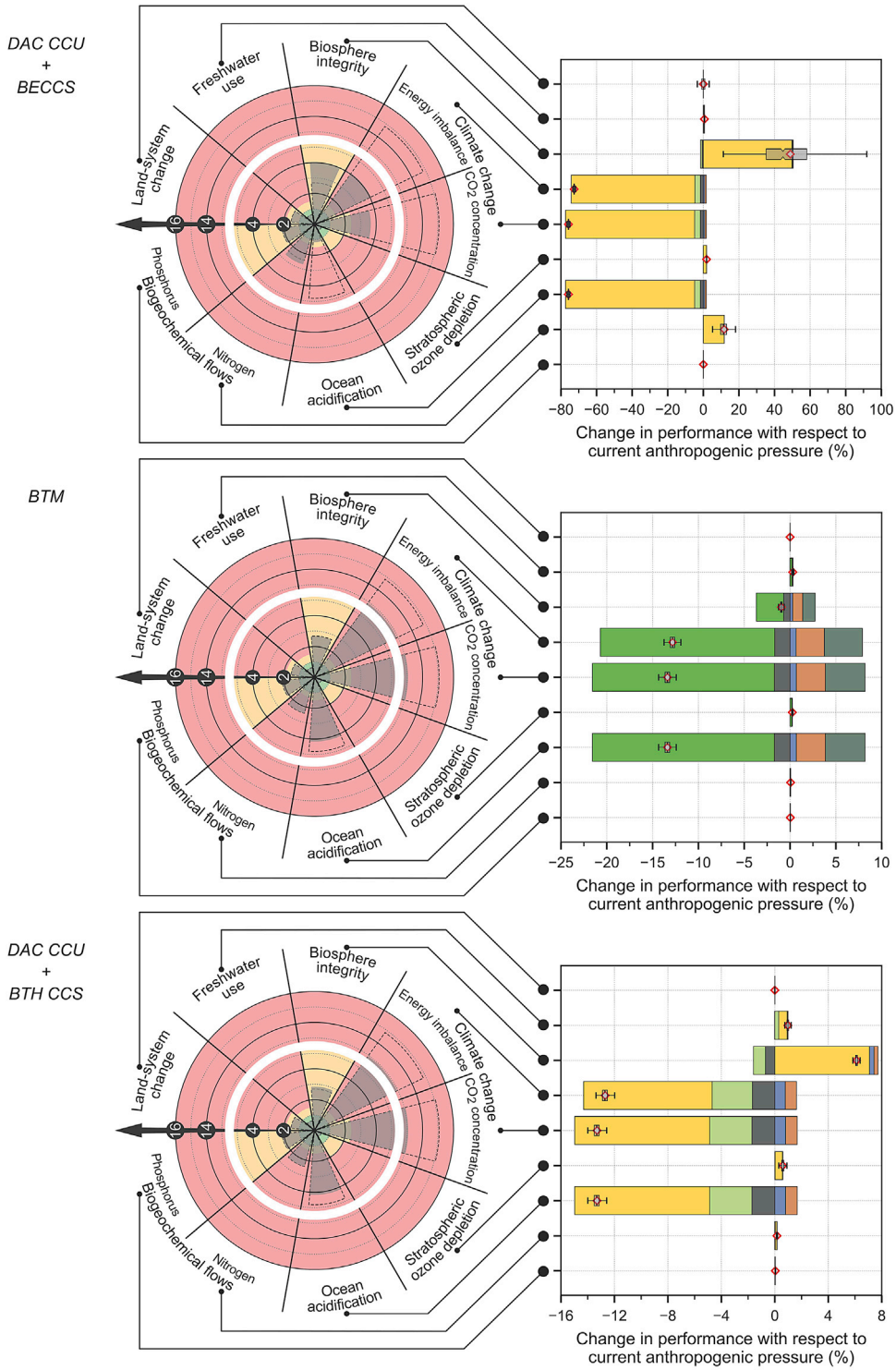
The analysis of the share of the global SOS occupied by each scenario (central results in red-green color in Figure 3), however, reveals the pitfalls of electrolytic H_2 from BECCS. Notably, this technology would pose threats to the biodiversity PB (133%–136% of the maximum global allowable budget) and, to a lesser extent, to the nitrogen flow (28%–29%). More precisely, the BECCS scenarios would improve the global PB footprint and provide ecological gains in the carbon-related PBs (negative shares of the SOS due to the CO_2 removed, leaving extra room for other sectors to operate within these PBs more flexibly). However, these scenarios would require more than 1.3 planet Earths to operate (omitting the impact of the remaining economic sectors). This high impact on biosphere integrity, therefore, makes them unsustainable despite their very low carbon footprint.

Similarly, the *BTH CCS* scenarios (relying on H_2 from biomass) would also exert high pressure on biodiversity, with shares of the SOS between 18%–22%, which calls into question their environmental sustainability. The remaining PBs in the *BTH CCS* scenarios always lie below 1.37%, attained in the *NG CCU + BTH CCS* scenario in the nitrogen flow PB due to the use of fertilizers (further discussed in Note S4). Among the remaining scenarios, the *DAC CCU + Nuclear* scenario would be easier to deploy in tandem with other PB mitigation strategies (all SOS shares < 1.72%, maximum attained in freshwater use), followed by *DAC CCU + Wind* (<2.28%, maximum in nitrogen flow PB), and finally by *DAC CCU + Hydro* (<6.15%, maximum in biosphere integrity). Notably, none of the alternative scenarios investigated would improve the *Fossil* scenario in all of the PBs simultaneously (i.e., there is no alternative win-win scenario), which evidences the unavoidable trade-offs between the Earth systems.[30]

We next focus on six representative scenarios selected from the total set of alternative scenarios (Figures 3 and S8) to shed further light on the global changes in performance (relative to the *Fossil* scenario) and associated drivers (Figures 4 and 5): two scenarios based on fossil CO_2 (currently available in power plants) combined with H_2 powered by wind, representing a potential interim solution (*Coal CCU + Wind*, *NG CCU + Wind*); one equivalent scenario based on DAC (*DAC CCU + Wind*), which (relative to the former two) could be regarded as a longer-term solution (Figure 4); and three bio-based scenarios

Figure 4. Performance of the *DAC CCU + Wind*, *NG CCU + Wind*, and *Coal CCU + Wind* scenarios satisfying the demand of platform chemicals in 2020

Polar charts on the left provide the global anthropogenic pressure on every PB associated with each of the three selected CO_2-based scenarios. Bar charts on the right show the breakdown of the changes in global performance attained by replacing the *Fossil* scenario with the corresponding alternative scenario, where negative bars indicate a relative improvement and positive ones denote a relative worsening. Boxplots over the bars indicate the variation in performance considering the uncertainty associated with the inventory data, with whiskers excluding outliers according to the 1.5 interquartile rule (experimental procedures). See also Figures S2–S4.



(legend on next page)

relying on various biomass resources encompassing agricultural residues, a dedicated bioenergy crop and forestry residues (Figure 5) and differing in whether the biomass would be used only as H_2 source (*DAC CCU + BTH CCS* scenario using poplar) as carbon feedstock and H_2 source (*BTM* scenario using straw) or only as an energy source (*DAC CCU + BECCS* using woodchips).

Analyzing first the changes in the Earth-system processes at a global scale, we find that the *NG CCU + Wind* and *Coal CCU + Wind* scenarios would worsen the global transgression in all the PBs, including the carbon-related ones (Figure 4). Conversely, the climate change and ocean acidification PBs would improve in the remaining four scenarios, with the largest reductions corresponding to *DAC CCU + BECCS* (between −72.58% and −75.78%), followed by *BTM* (between −12.82% and −13.38%), then *DAC CCU + BTH CCS* (between −12.69% and −13.30%), and finally *DAC CCU + Wind* (between −1.61% and −1.07%). The improvements in these four scenarios would be attained at the expense of shifting burdens toward the remaining PBs, except for the biosphere integrity impact that would diminish in the *DAC CCU + Wind* and *BTM* scenarios (i.e., −0.34% and −0.95%, respectively). The collateral damage would be particularly critical in the *DAC CCU + BECCS*. Notably, this scenario would worsen the most the biosphere integrity (+48.86%), followed by the nitrogen flow (+11.71%, further discussion in Note S3), and then the other PBs (below +1.82% of increase, with negligible collateral damage in the phosphorus flow and land-system change PBs). In contrast, the detrimental side effects in the *DAC CCU + BTH CCS* and *BTM* scenarios would be of much less concern, always below +1.00% for all the PBs except for the biosphere integrity in the *DAC CCU + BTH CCS,* which would worsen +6.12%.

The global changes in PB performance are linked to the substitution of the current *Fossil* scenario and the addition of alternative feedstocks and utilities (bar charts in Figures 4 and 5 and breakdown per kg of platform chemical; Figures S2–S7). Analyzing these contributions and focusing on the CCU scenarios first (Figure 4), we find that in the *NG CCU + Wind*, *Coal CCU + Wind*, and *DAC CCU + Wind* scenarios, the primary source of impact worsening the transgression levels in all of the PBs is often the H_2. This contribution is followed by the utilities of the methanol plant and the MTO and MTA processes and then the captured CO_2. The DAC CO_2 was modeled as a negative flow (removal of CO_2 from the atmosphere); consequently, its impact contribution in the *DAC CCU + Wind* scenario to the carbon-related PBs and the biosphere integrity is negative (−3.11% on average in the former PBs and −0.90% in the latter).

The large impact of H_2 is explained by the high energy and water requirements of water electrolysis (63 kWh kg^{-1} H_2 and 11 kg H_2O kg^{-1} H_2, respectively). Notably, despite its low carbon footprint, the production of wind turbines and the construction of wind farms require metallic materials (e.g., glass fiber) and emit pollutants such as nitrogen compounds, phosphates, and substances causing ozone smog formation. Improvements in the electrolyzer efficiency and siting new wind projects in locations with favorable load factors could mitigate these impacts.[41] Concerning the utilities for the methanol, MTO and MTA plants, generating power on-site by, for example, burning the flue gas or buying electricity from a greener grid, could reduce the environmental impacts of the power inputs.

In the bio-based scenarios relying on CO_2 captured (*DAC CCU + BECCS* and *DAC CCU + BTH CCS* in Figure 5), H_2 would again emerge as the main contribution (in absolute value) toward most of the PBs. The contribution of utilities (electricity and heating) would be, in general, much lower, worsening mainly the carbon-related PBs and the biosphere integrity PB. The H_2 powered by BECCS (*DAC CCU + BECCS* scenario) would lead to the most drastic reductions in climate change energy imbalance, climate change CO_2 concentration, and ocean acidification (−69.50%, −72.57%, and −72.58%, respectively), as well as to the most severe burden shifting toward biodiversity and the nitrogen flow (+49.82% and +11.67%, respectively). Similarly, H_2 from biomass (*DAC CCU + BTH CCS*) would also worsen biodiversity loss (to a lesser extent, +7.08%), while improving climate change energy imbalance, climate change CO_2 concentration, and ocean acidification (−9.61%, −10.10%, and −10.10%) and slightly worsening the other Earth-system processes (<+0.64%).

Delving into the technical features of these scenarios, we find that the large reductions in the carbon-related PBs linked to the H_2 from BECCS are due to the carbon-negative electricity from wood chips powering water electrolysis (−1.59 kg CO_2 kWh^{-1}). This scenario, however, exacerbates the biosphere integrity PB substantially due to its large land-occupation requirements (linked to the wood feedstock, i.e., forests with intensively extractive land use, contributing strongly to the impact in biosphere integrity, >99%). Furthermore, the *DAC CCU + BTH CCS* scenario reduces the impact on climate change and ocean acidification because the CO_2 uptake during poplar growth, together with its long-term sequestration in geological sites, leads to a net-negative carbon balance (−13.77 kg CO_2 kg^{-1} H_2). However, this carbon sequestration cannot offset the impact of land use, so biodiversity loss worsens overall.

Finally, due to the CO_2 uptake during photosynthesis, the biomass (straw) in the *BTM* scenario would improve climate change energy imbalance, climate change CO_2 atmospheric concentration, ocean acidification, and biosphere integrity (−12.82%, −13.38%, −13.38%, and −0.95%, respectively). On a cradle-to-grave basis, however, these ecological gains would become much smaller because, without permanent carbon sequestration, the *BTM* scenario would be at most carbon neutral.

Figure 5. Performance of the *DAC CCU + BECCS*, *BTM*, and *DAC CCU + BTH CCS* scenarios satisfying the demand of platform chemicals in 2020

Polar charts on the left provide the global anthropogenic pressure in every PB associated with each of the three selected bio-based scenarios. Bar charts on the right show the breakdown of the global performance changes attained by replacing the *Fossil* scenario with the corresponding alternative scenario, where negative bars indicate a relative improvement, and positive ones denote a relative worsening. Boxplots over the bars indicate the variation in performance considering the uncertainty associated with the inventory data, with whiskers excluding outliers according to the 1.5 interquartile rule (experimental procedures). See also Figures S5–S7.

Implications of shifting to renewable carbon in the chemical industry

After highlighting the environmental benefits of the defossilization of chemicals, we next analyze its technical, economic, and sociopolitical implications, considering the links with the power sector and the availability of feedstocks. The global deployment of the CCU routes would require (regardless of the carbon and H_2 source) 2,107 Mt year^{-1} of CO_2 and 287 Mt year^{-1} of H_2 in addition to substantial electricity and heating requirements. The total CO_2 emissions worldwide from coal and natural gas plants amounted to 13,050 and 1,888 Mt year^{-1} in 2018,[42] respectively, whereas DAC can be regarded as a source of unlimited carbon, constrained only by energy availability and costs.

Furthermore, the routes relying on biomass resources would require 2,511 Mt year^{-1} of straw (*BTM* scenario), 10,407 Mt year^{-1} of poplar (*BTH CCS* scenarios), and 18,717 Mt year^{-1} of wood chips (*BECCS* scenarios). According to global estimates, there would be enough agricultural residues in 2050[43,44] to cover the demand of straw residues in the *BTM* scenario (34%–158% of the amount demanded) but not enough wood chips to meet the biomass demand in the *BECCS* scenarios (less than 38%[45]). Moreover, the potential of dedicated energy crops like the poplar short-rotation coppice in the *BTH CCS* scenarios will depend on the land availability and its suitability for the crop (yield, i.e., kg ha^{-1}). Considering the degraded or marginal land availability at a global scale, both unsuitable for agriculture, the technical potential for dedicated biomass production would be at most 110 EJ year^{-1},[43] placing the most optimistic estimates at 58% of the land required by the poplar plantations that would be needed in the *BTH CCS* scenarios.[45] Competing uses from other sectors could lower these potentials, whereas considering surplus agricultural land (or abandoned land) would make additional land resources available for bio-energy plantations.[43]

Moreover, the bio-based alternatives with CCS would face logistic challenges (i.e., BECCS and BTH CCS), such as the availability of geological storage sites in the proximity of the biomass resources. Theoretical global estimates for storage (i.e., 35,000 Gt CO_2[45,46]) suggest that there would be sufficient capacity to store the CO_2 captured for a long period (e.g., more than 1,140 years in the *DAC CCU + BECCS* scenario, considering that 30.70 Gt CO_2 would be annually stored). Nevertheless, the storage availability could be affected by physical and practical constraints,[45] ultimately hampering the deployment of the scenarios involving CCS.

Overall, the fossil CO_2 requirements could be covered by retrofitting with CCS systems the existing coal and natural gas power plants. However, these scenarios would need H_2 from biomass with CCS or H_2 powered by BECCS to achieve carbon neutrality (or even yield a negative balance). Using biomass as a carbon source seems appealing (*BTM* scenario); however, regionalized assessments providing more accurate estimates of the biomass availability and its performance would be needed to gauge its true potential. In contrast, this regional dimension might be less critical for DAC, provided suitable locations with high-capacity factors are selected for the renewable source powering its operation. Hence, biomass combined with DAC could help to close the carbon loop in the chemical industry. This would be accomplished by using atmospheric carbon as the carbon source for chemicals and releasing it back in the end-use phase. Removing 2,107 Mt of CO_2 via DAC would, however, require around 771 TWh year^{-1} of electricity and 11 EJ year^{-1} of heating, representing 2.9% and 8.5% on the global final electricity and energy supply (from natural gas) in 2018, respectively.[47] Better adsorbents for CO_2 removal and the use of biomass or waste heat to power DAC would make it more competitive.

With regard to the H_2 requirements, its electrolytic production would need 18,139 TWh year^{-1}, which should not be entirely covered either by electricity from the grid (resulting in chemicals with a larger carbon and PB footprint) or via BECCS (due to the large impact on biodiversity[48]). This electricity demand represents more than seven times the world prospects for net power generation from wind in 2040[42,47] and more than four times the expected BECCS capacity from wood chips. Therefore, the global transformation of the petrochemical industry relying on electrolytic H_2 would require a substantial expansion of renewables. In this context, dedicated microgrids integrating a portfolio of technologies could power chemical clusters while ensuring the desired environmental and economic performance levels. Using biomass gasification coupled with CCS would reduce the large energy requirements of the electrolytic H_2. However, a detailed regionalized assessment accounting for biophysical limitations and sustainability criteria should be performed on a case-by-case basis, considering the location of all the life-cycle activities. Regional impacts should not be overlooked as they could vary greatly across regions with different characteristics (e.g., regional functioning of the water cycle and water stress indicators[49] and assimilation capacity for nitrogen emissions). Furthermore, the competition for H_2 across sectors should not be underestimated because H_2 is a versatile energy carrier with applications in energy supply and transportation.[50]

Regarding the economic implications, at current prices, the CO_2-based chemical industry would imply sharp increases in total costs (more than three-fold in the *Coal CCU + Wind*, *NG CCU + Wind*, and *DAC + Wind CCU* scenarios, in comparison with the *Fossil* scenario) (Figure 6), due to the expensive green electrolytic H_2[11] (breakdown by feedstocks and utilities in Figure S9). Notably, the CCU scenarios relying on CO_2 from DAC are significantly more expensive. This higher cost is due to its larger energy needs linked to the lower CO_2 concentration in the air than in the flue gas from power plants (e.g., 0.05–0.06 USD kg^{-1} CO_2 in coal power plant versus 0.16–0.23 USD kg^{-1} CO_2 from DAC). The increase in costs would be more pronounced for aromatics due to their lower yields per kg of methanol, i.e., around four times more expensive than the fossil-based analog. Even under the current most optimistic cost data, the cost of the *CCU* scenarios would be more than double (relative to the fossil analog) and around six-fold in the most pessimistic case (error bars in Figure 6 and details in experimental procedures). The *DAC CCU + BECCS* scenario would be the most expensive (six-fold increase) due to the costly electrolysis based on BECCS (i.e., 11.0–13.2 USD kg^{-1} H_2) and the currently expensive DAC. The economic performance would improve substantially by replacing the expensive electrolytic H_2 by H_2 from biomass with CCS (*DACC CCU + BTH*, 2.3- to 2.9-fold increase),[51] and further so in the *BTM* scenario, which could even outperform the *Fossil*

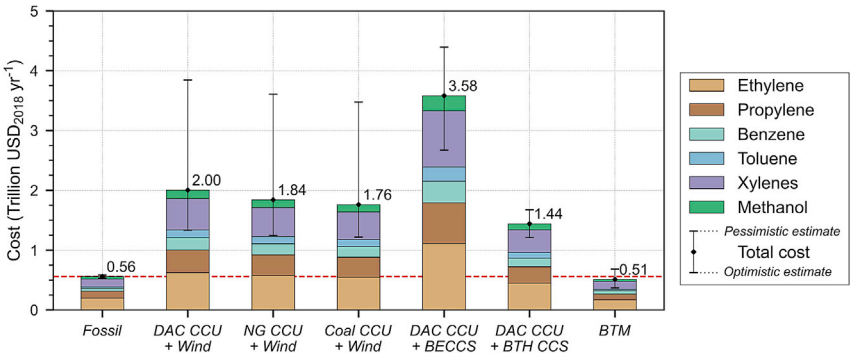


Figure 6. Global costs of the chemical industry for the scenarios in 2020

Each stacked bar, which corresponds to a different scenario, provides the cost breakdown into platform chemicals. Error bars depict the pessimistic and optimistic cost estimates according to values found in the literature[41] (see experimental procedures for details on the sensitivity analysis). See also Figure S9.

scenario. Hence, the biomass utilization routes emerge as economically appealing.

Future trends could strongly affect the economic viability of the scenarios. For example, the cost of electrolytic H_2 from wind is expected to drop significantly, most likely reaching 0.9–2.5 USD kg^{-1}. Improvements in the electrolyzers and a decline in the levelized cost of electricity, realized by exploiting the most suitable locations for wind and solar farms and by procuring the excess of renewable energy at near-zero marginal prices,[11,41,52] will likely drive this cost reduction. Reaching the break-even point of the CCU chemicals would require a H_2 cost of 1.3 and 1.0 USD kg^{-1} H_2 for the *Coal CCU + Wind* and *NG CCU + Wind* scenarios, respectively, and 0.45 USD kg^{-1} for both the *DAC CCU + Wind* and *DAC CCU+BECCS* scenarios; such a low cost might be unlikely in the foreseeable future but possible for favorable regions. Furthermore, reductions in the cost of DAC[8,53] and CO_2 capture from point sources, linked to enhanced capture technologies and/or the use of CO_2-rich gaseous waste industrial streams, could make CCU routes economically more appealing. Finally, the cost of the biomass-based scenarios (*DAC CCU + BTH CCS* and *BTM*) could vary depending on future technological improvements and on the biomass cost, which will be affected by future market trends and policies.

The defossilization of chemicals might also face social acceptance and political barriers. The global value chain of the defossilized chemicals would require deploying new infrastructure and establish cross-border cooperation mechanisms. The latter would be needed to coordinate the CO_2 capture, biomass collection, power facilities, and production sites, which would be geographically dispersed to exploit regional advantages. Public acceptance issues and regulatory constraints might also hamper the massive deployment of wind farms or dedicated biomass production, often perceived as a threat to food production.

In view of this, market and non-market mechanisms and new policies will be needed to encourage the transition toward the defossilized chemical industry. Incentives such as technologies mandates, subsidies, or carbon-neutrality (or negative-emissions) targets could help to promote the alternative routes.[54,55] Equity-based allocation strategies for sharing the SOS at different scales (e.g., national, sector, business)[56] could also be established, together with tradable permit mechanisms beyond GHG emissions that would focus on the main drivers of the PBs' transgression (i.e., the main resources and emissions to air, soil, and water exerting pressure on the Earth-system processes). Moreover, environmental taxes based on negative externalities—"Pigouvian" price-based instruments—could help to reduce effluents and resource usage threatening the PBs.[32] In this context, existing statistical frameworks, like the one developed by the European Commission, the OECD, and the International Energy Agency, could be used as the starting point to translate resources and emissions to air and water linked to the Earth systems of the PBs into economic taxes.[57]

DISCUSSION

Here, we assessed the implications on the resilience of the Earth system of emerging pathways to replace fossil carbon by renewable carbon in the chemical industry. Our results are affected by limitations stemming from methodological LCA choices (e.g., scope of the analysis and allocation methods), the simplifications and assumptions of the PB assessment methods (e.g., omission of regionalized PBs and PBs yet to be quantified, and assumptions affecting the nitrogen flow and biosphere integrity PB calculations), and data quality (Note S3). Acknowledging these limitations, our work has a wide range of relevant implications for sustainable decision and policy-making. First, we demonstrated that environmental assessments should embrace a wide range of impacts quantified at the global level. Standard LCA metrics should therefore be complemented with absolute sustainability indicators based on the PBs, like the PB footprint proposed herein and the shares of the SOS occupied by an activity, to assess the performance relative to an absolute reference system as defined by the PBs.[26]

Our results uncover the potential threats of maintaining the current fossil-based petrochemical industry, which simply requires an excessive ecological budget (i.e., standalone a quarter of the SOS available for all the economic activities). Shifting to renewable carbon could reduce the damage to the core critical climate change-related PBs, thereby leaving room for other hard-to-abate economic activities. However, defossilization efforts could exacerbate the biosphere integrity PB severely in some seemingly appealing scenarios. Notably, the collateral damage would be particularly critical in scenarios relying on biomass feedstocks as power source to produce electrolytic H_2 and, to a lesser extent, in those using biomass as hydrogen source, mostly due to the high land-use requirements. Nevertheless, the shift to renewable carbon in chemicals production could significantly contribute to operating safely within PBs by selecting the appropriate technologies to mitigate the adverse side effects.

The effective transition toward the defossilized chemical industry could combine CO_2-based and bio-based alternatives to exploit their complementary strengths (wider availability and lower costs and impact, depending on the biomass source, respectively). There is no technological silver bullet based on renewable carbon to make the chemical industry fully sustainable, which calls for a portfolio of alternatives to be optimized considering technological features, market forces, and other regional data. Notably, the deployment of alternative chemical production pathways should consider the precise location of the facilities, because some impacts across chemical supply chains might be region specific.[58,59]

In the short term, CCU at point sources could contribute to decarbonizing current energy mixes, more so if combined with carbon-negative H_2 from biomass with CCS. The CO_2 could be captured from existing coal or natural gas power plants or, alternatively, from other hard-to-decarbonize industrial activities such as cement, steel, or aluminum production.[1] This interim strategy would enable the development of the necessary infrastructure to ultimately deploy the DAC scenario, currently more expensive and unproven at scale but with the potential to ultimately close the carbon loop in chemicals production.

In the longer term, after decarbonizing the power sector, the future chemical industry we envision would mostly rely on renewable carbon from DAC or biomass. The use of CO_2 from the atmosphere, captured either by engineered processes or natural photosynthesis, would help to virtually close the carbon loop in the chemical sector and enable a net-zero CCU system (circular economy). Hence, biomass utilization emerges as an attractive option to defossilize the chemical industry, either directly to produce methanol or to generate H_2 to activate the CO_2 molecule, which seems environmentally and economically appealing and relies on mature technologies. However, the suitability of these bio-based scenarios will strongly depend on the biomass type and location. These two factors will define the environmental and economic performance as well as deployment potential. The latter will be constrained by the domestic biomass availability and the increasing competition for biomass resources and land with the food sector and other industrial uses.

In contrast, the CCU pathways relying on CO_2 from DAC will face significant barriers to scaling at present, mainly due to their high energy needs and associated costs. These drawbacks could be overcome (to some extent) by technological improvements and the selection of alternative energy sources to power its operation, e.g., low-carbon waste heat sources. Nevertheless, DAC needs to be demonstrated at scale to reduce the uncertainties surrounding its future deployment potential and costs, which will most likely require targeted support.

Regardless of the carbon source, the defossilization of the chemical industry will face multiple technical, economic, and sociopolitical challenges. More efficient electrolyzers, cheaper renewables, the selection of favorable locations for the H_2 and biomass projects, and the sustainable exploitation of biomass resources could significantly help to overcome the main barriers. In light of the risks of transgressing the PBs, tailored policy instruments and measures would be required to incentivize more sustainable alternatives and a quick transition toward renewable carbon. Technology mandates or subsidies rooted in scientific studies could help to deploy the best pathways to sustainable development. Alternatively, taxes based on externalities could also be considered to penalize environmental burdens threatening the PBs, and certification and labeling for renewable carbon-based products could also promote more sustainable chemicals and reach environmentally conscious consumers.

Identifying effective solutions to global challenges is crucial for sustainable development. In this context, our bottom-up PB-based analysis and biosphere integrity PB-LCA method could be applied to other emerging technological roadmaps within the chemical industry and beyond to quantify the impact of anthropogenic activities at different scales toward reversing or avoiding the transgression of the PBs. The new methods, findings, and rich datasets presented in this work will, therefore, help to open up new avenues for the absolute sustainability assessment of technological decisions linked to grand challenges. By adopting a global sustainability perspective, results will be more easily communicated to scientists, decision-makers, and the wider society, thereby underpinning sustainable development in academia, businesses, and governance.

EXPERIMENTAL PROCEDURES

Resource availability

Lead contact

Further information and requests for resources should be directed to and will be fulfilled by the lead contact, Gonzalo Guillén-Gosálbez (gonzalo.guillen.gosalbez@chem.ethz.ch).

Materials availability

This study did not generate new unique materials.

Data and code availability

All the data used in this study can be found from the references mentioned in the experimental procedures. Input and resulting datasets generated during the current study are publicly available online at Galán-Martín et al.[60]

Scenario definitions

Our analysis considers 51 different scenarios. The *Fossil* scenario, taken as a baseline, represents the current petrochemical industry converting fossil resources into chemicals. Additionally, we model 50 alternative scenarios (see Note S1, Figure S1, and Table S1 for the acronyms and description of the scenarios) relying on green methanol as intermediate. Methanol can be obtained through biomass gasification (*BTM* scenario) or catalytic hydrogenation of CO_2, captured either from point sources at coal or natural gas power plants or directly from the air (the *Coal CCU*, *NG CCU*, or *DAC CCU* scenario, respectively). Furthermore, H_2 can be produced via steam methane reforming with CCS (*SMR CCS* scenario), from biomass gasification with CCS (*BTH CCS* scenario), or via water electrolysis powered by different energy sources. For the electrolytic routes, we consider seven power alternatives, including five standalone technologies, namely, onshore wind, solar photovoltaic, nuclear, hydroelectricity and BECCS, and power from the grid provided with either the current or future electricity mix. These scenarios are labeled as *Wind*, *Solar PV*, *Nuclear*, *Hydro*, *BECCS*, *Current mix*, and *Future mix*, respectively.

For all the alternative scenarios, we consider that the power grid covers the electricity demand of the processes in the foreground system (over which decision makers have a certain level of control), excluding the electricity for water electrolysis in the *Wind*, *Solar PV*, *Nuclear*, *Hydro*, and *BECCS* scenarios. This power grid corresponds to either the current or future electricity mix (modeled on the basis of the Stated Policies Scenario or Sustainable Development Scenario, respectively, provided in the World Energy Outlook).[40] The main set of results discussed in the manuscript are based on the current mix. The future mix results presented in Note S2 are only briefly discussed. We model the electricity requirements in the background system with the default data in Ecoinvent v3.5.[61] An additional discussion on the main assumptions and limitations can be found in Note S3.

Six platform chemicals are considered, i.e., ethylene, propylene, benzene, toluene, xylenes, and methanol. These petrochemicals are precursors of a

myriad of other chemicals and materials, such as thermoplastics, fuels, solvents, and polymers, among others. A cradle-to-gate scope is adopted, covering the procurement of raw materials, generation of utilities, and direct emissions and wastes of the main production processes. Downstream routes from platform chemicals to other fine and bulk chemicals are the same across scenarios, so adding them would add no discriminatory power to the analysis.

In the first scenario, the *Fossil* scenario, platform chemicals are obtained from fossil-based resources, i.e., the business-as-usual petrochemical industry. Here, methanol is produced from natural-gas-based synthesis gas via steam reforming. At the same time, the olefins (ethylene and propylene) and aromatics (benzene, toluene, and xylenes) are generated via steam cracking of naphtha, ethane, or LPG or by catalytic reforming of naphtha.

The alternative scenarios convert green methanol into olefins (via MTO) and aromatics (via MTA). All the technologies considered in the alternative scenarios show a high TRL (>8), implying that the system has been completed and qualified or has been proven in an operational environment.[4] Green methanol can be obtained via biomass gasification or by the reaction of CO_2 with H_2. The *BTM* scenario considers the production of methanol from biomass gasification (straw from agricultural activities).[62] The *SMR CCS* scenarios consider a reference process for steam reforming of natural gas coupled with a CCS system based on CO_2 absorption with amines, followed by compression and injection in exhausted oil fields.[63] The *BTH CCS* scenarios produce H_2 from short-rotation poplar biomass through gasification coupled with CO_2 capture based on membranes.[64] The *Coal CCU* scenarios consider a post-combustion CO_2 capture technology at a coal-fired power plant based on chemical absorption with a monoethanolamine (MEA).[65] The *NG CCU* scenarios consider a conventional combined-cycle natural-gas-fired power plant with installed pre-combustion CO_2 capture at the exit of an auto-thermal reformer[66] and CO_2 capture via the same chemical absorption with MEA as in the previous case. Finally, in the *DAC CCU* scenarios, the CO_2 is directly captured from the air by an industrial DAC system with an aqueous sorbent.[67]

Because of space limitations, the main manuscript focuses on six representative alternative scenarios: CO_2 captured in coal and natural gas power plants combined with electrolytic H_2 from wind power (*Coal CCCU* + *Wind* and *NG CCU* + *Wind*, respectively), CO_2 captured from the air, and electrolytic H_2 generated from wind or BECCS power (*DAC CCU* + *Wind* or *DAC CCU* + *BECCS*, respectively), CO_2 from air and H_2 from gasification of biomass with CCS (*DAC CCU* + *BTH CCS*), and the *BTM* scenario.

Characterization of chemical routes

For each alternative route, we carry out a simplified technical, environmental, and economic assessment considering its primary feedstocks and utility requirements, i.e., the carbon and H_2 source and the electricity and heating needs. Data sources are available in Galán-Martín et al.,[60] and a description of the main assumptions and limitations of our analysis is included in Note S3.

For the environmental evaluation, the general LCA methodology based on the ISO 14040/44 framework is followed.[68,69] In phase one, the goal and scope of the analysis are defined. The functional unit is a given annual demand for chemicals to be met (Table S1 in Galán-Martín et al.[60]). We adopt a cradle-to-gate scope that omits the downstream conversion routes transforming the platform molecules into other chemicals under the assumption that these further processing pathways would remain unaltered in the alternative scenarios.

In step two, the life-cycle inventory (LCI), all the input and output flows associated with the production of chemical *c* are quantified (i.e., energy, raw materials, natural resources, by-products, wastes, and emissions). The LCI integrates information of the foreground and background systems. The former data, retrieved from the literature, characterizes the main processes (i.e., methanol production, MTO, and MTA) as well as the procurement of H_2, CO_2, and biomass. On the other hand, data of the background system, used to model the surrounding processes supplying feedstocks and utilities to the main ones, are retrieved from Ecoinvent v3.5.[61] In mathematical terms, given a set of scenarios *S*, the LCI elementary flow *e* associated with the production of chemical *c* in scenario *s* is computed from the corresponding consumption rate of utilities *u* and raw materials *r* (belonging to sets *U* and *R*, respectively) according to Equation 1:

$$LCI_{c,e,s} = \sum_{u\in U} LCI^{UTI}_{u,e,s}\cdot \upsilon_{u,c,s} + \sum_{r\in R} LCI^{RAW}_{r,e,s}\cdot \mu_{r,c,s} + LCI^{DIR}_{c,e,s} + LCI^{WASTE}_{c,e,s}$$
$$\forall c\in C, e\in E, s\in S, \qquad \text{(Equation 1)}$$

where $LCI_{c,e,s}$ denotes the total amount of LCI elementary flow *e* per unit of chemical *c* in scenario *s* (e.g., m^3 of water per kg of methanol in the *DAC CCU* + *Wind* scenario); $\upsilon_{u,c,s}$ and $\mu_{r,c,s}$ are parameters representing the unitary consumption of utility *u* and raw material *r* per unit of chemical *c*, respectively (e.g., kWh per kg of methanol or kg of H_2 per kg of methanol) in each scenario *s*; $LCI^{UTI}_{u,e,s}$ and $LCI^{RAW}_{r,e,s}$ denote the LCI elementary flow *e* per unit of utility *u* and raw material *r* associated to the background system, respectively (e.g., kg of CH_4 per kWh or per kg of H_2), and $LCI^{DIR}_{c,e,s}$ and $LCI^{WASTE}_{c,e,s}$ are the elementary flows (i.e., direct emissions and waste, respectively) of the foreground system. To compute the LCIs, we first quantify the LCI elementary flows embodied in CO_2, H_2, and biomass, then estimate the LCI elementary flows of methanol, and finally determine the LCI elementary flows for the remaining platform chemicals. For the *BTM* scenario, we use aggregated data of the biomass to methanol process.[62] Background data (LCI elementary flows) for utilities and raw materials ($LCI^{UTI}_{u,e,s}$ and $LCI^{RAW}_{r,e,s}$) were retrieved from Ecoinvent v3.5 accessed via SimaPro v9.0.[70] All data for the raw materials and utility requirements and life cycle inventories used in this study can be found in Galán-Martín et al.[60]

In phase three, these LCI elementary flows ($LCI_{c,e,s}$) are converted into impacts on the control variables of the PBs by using a set of characterization models, as discussed next. Additionally, we also assessed the impacts of the chemicals with the midpoint category indicator for "Climate change" of the well-established ReCiPe 2016[71] LCA method considering a Hierarchist perspective (Figures 3 and S8). We also considered an end-use phase scenario accounting for the oxidation to CO_2 of the carbon contained in the six platform chemicals, which amounts to 1.79 Gt CO_2-eq ("cradle-to-grave" values reported in Figures 3 and S8).

Finally, in step four of the LCA methodology, the results are interpreted, and recommendations are made. Here, we quantify the change in performance in each control variable compared to the *Fossil* scenario and further analyze the shares of each scenario in the SOS defined for every PB.

The economic characterization of the chemical routes was performed as follows:

$$PC_{c,s} = \sum_{u\in U} C^{UTI}_{u,s}\cdot \upsilon_{u,c,s} + \sum_{r\in R} C^{RAW}_{r,s}\cdot \mu_{r,c,s} \quad \forall c\in C, s\in S \qquad \text{(Equation 2)}$$

Equation 2 provides the unitary production cost of a chemical *c* in each scenario *s* ($PC_{c,s}$), expressed in USD_{2018} per kg of chemical. This cost is computed as the summation of the costs of utilities and raw materials consumed by the chemical process. The capital costs of the methanol, MTO, and MTA processes are here omitted to yield a lower bound on the cost. Hence, here we work under the assumption that in petrochemicals the capital costs are often lower than the operating costs, which are driven mostly by the raw materials and, to a lesser extent, utilities consumption.[11,72] The exception to this simplification is the *BTM* scenario, where the CAPEX could represent as much as 50%–55% of its total production costs[73] and therefore should be considered. $C^{UTI}_{u,s}$ and $C^{RAW}_{r,s}$ correspond to the unitary cost of the utilities *u* and raw materials *r* (e.g., USD_{2018} per kg of CO_2), respectively, for each scenario *s*. Again, this equation is applied recursively to estimate first the cost of methanol, and then the cost of the platform chemicals. The costs of CO_2, H_2, and biomass were retrieved from the literature.

Cost data were sourced from various literature sources (see Galán-Martín et al.[60]), while consumption rates of utilities and raw materials ($\upsilon_{u,c,s}$ and $\mu_{r,c,s}$) were estimated as explained below.

For methanol production via biomass gasification (*BTM* scenario), we retrieved the unitary consumption rates of inputs from Liu et al.[62] For methanol production from CO_2 hydrogenation, the unitary consumption of H_2 and CO_2 together with the electricity and heating requirements were taken from Perez-Fortes et al.[21] The data for the production of H_2 via *SMR CCS* scenarios were sourced from Dufour et al.[63] Data for H_2 production from biomass with CCS (*BTH CCS* scenarios) were taken from Susmozas et al.,[64] and for the poplar biomass consumed by the process, the data were sourced from Gasol et al.[74]

For the water electrolysis routes, the utilities and raw materials requirements were taken from an LCA study by Lee et al.[75] based on H_2 production via water electrolysis powered by wind. According to the authors, producing 1 kg of H_2 requires 11 kg of water and 62.72 kWh. Additionally, we added 0.44 kWh of electricity per kg H_2 to compress the H_2 from 8.3 bar to 30 bar at 25°C to be entirely consistent with the feeding conditions of the methanol process. Similarly, for the SMR CCS and the BTH CCS delivering the H_2 at 22 bar, we added 0.16 kWh per kg of H_2 to compress it to 30 bar. Moreover, we consider H_2 storage to ensure the continuous operation of the methanol plant consuming H_2 produced from intermittent wind and solar power. Notably, once produced intermittently in the polymer electrolyte membrane (PEM) electrolyzer, H_2 is compressed to 200 bar and stored,[76] either in caverns or in standard steel tanks using a three-stage H_2 compression. Due to the global scope of our work and because the dynamic profile of wind and solar is region specific, the amount of H_2 stored is estimated considering typical values of the capacity factor (i.e., 0.34 and 0.18 for wind and solar PV, respectively) and the total annual operating h. Accordingly, we added 1.77 kWh per kg of H_2 for the wind and solar scenarios, which represents only 2.79% of the total energy embodied in the H_2 for wind and solar, respectively. All the compression requirements were estimated with Aspen HYSYS v9.0.[77]

Data on CO_2 capture were defined as follows. Data for the *Coal CCU* scenarios were taken from the work by Iribarren et al.[65] based on a coal-fired power plant with post-combustion captured of CO_2 with chemical absorption with MEA. For consistency with the CCU process, which requires a lower input pressure compared to the carbon capture and storage analog, these data were adjusted by removing the last compression stage to deliver CO_2 at around 1 bar (decompression from 187 bar to 1.2 bar, which corresponds to the pressure of the stream fed to the first compression stage[65]). This adjustment reduces the energy embodied in the captured CO_2. For the *NG CCU* scenarios, the data were retrieved from Petrakopoulou et al.,[66] which considered a natural gas plant with an auto-thermal reformer and pre-combustion CO_2 capture with MEA. Again, for consistency, the data were adjusted by removing some compression stages (to save as much energy as possible), thereby delivering the CO_2 at around 1 bar (based on Petrakopoulou et al.,[66] the pressure was adjusted from 103 bar to 12.94 bar, whereas the remaining decompression energy is assumed to be lost). For the *DAC CCU* scenario, the work by Keith et al.[67] was considered, which reported real data of a DAC commercial plant from Carbon Engineering (~1 Mt CO_2 captured/year) considering a mono-functional process based on an aqueous KOH solvent. These data were also adjusted by subtracting the electricity required in the final compression stage (decompression from 151 bar to 1 bar). No additional compression for transporting the CO_2 from capture point sources to chemical plants was considered under the assumption that the methanol plant would be located near the CO_2 source. The CO_2 feedstock sourced from DAC is modeled as a negative output in the LCA as it results in a removal of atmospheric CO_2. Similarly, the biogenic CO_2 in the biomass inputs (i.e., wood pellets in the *BECCS* scenarios, poplar in *BTH CCS* scenarios and straw in *BTM* scenario) is also modeled as a negative entry because it is removed from the atmosphere during the biomass growth. Note that, on a cradle-to-gate basis, this could lead to a negative carbon footprint; however, only pathways with CCS can potentially lead to a negative balance on a cradle-to-grave basis.

For the MTO processes, data from Dutta et al.[78] was considered. To cover data gaps in the original reference, the electricity used in the refrigeration cycles of the MTO process (to cool the dry gas and remove H_2) was estimated considering the multi-stage compression refrigeration design proposed by Luyben.[79] Notably, the four grades of refrigerants in the original MTO process at −140, −115, −100 and −35°C were assumed to require a compression power of 6.3, 3.7, 2.4, and 1.9 MW of electricity per MW of cooling, respectively.[79]

We modeled the MTA processes based on Zhang et al.[80] Again, we translated the refrigeration needs (for distilling the aromatics mixture) into electricity consumption using the refrigeration cycles proposed by Luyben.[79]

For those multi-functional processes—where more than one product is obtained—the total raw materials and utility needs were allocated among the main product and associated by-products. This allocation concerns the CO_2 captured at coal and natural gas power plants, where net electricity is generated together with the CO_2 feedstock. Following recommendations for LCA studies on CCU, the CO_2 captured at power plants is treated as a co-product, i.e., a technical flow of CO_2 feedstock, and its embodied impacts are quantified via economic allocation.[81] Similarly, the economic allocation was applied to allocate the inputs (raw materials and utility consumption) and outputs (emissions and wastes) of the MTO and MTA processes among their co-products, as recommended in the literature[82,83] and shown in Equation 3:

$$AF_p = \frac{price_p \cdot \dot{m}_p}{\sum_{p' \in P} price_{p'} \cdot \dot{m}_{p'}} \quad \forall p \in P, \qquad \text{(Equation 3)}$$

where AF_p is the allocation factor for any valuable product p, i.e., the percentage of the total amount of raw materials and utilities consumed allocated to this product; and $price_p$ and $\dot{m}_p$ denote the unitary price (e.g., € kg^{-1} CO_2 or € kWh^{-1}) and the amount of co-product p produced, respectively (e.g., kg of CO_2 or kWh). Parameter AF_p is then multiplied by the total inputs and outputs of the process to calculate the percentage that is allocated to each product p. Prices data can be found in Galán-Martín et al.,[60] whereas mass flows were taken from the original references.

Bottom-up PB framework and biosphere integrity method

Our PB assessment combines (1) a new bottom-up approach to quantify the PB performance of a system that does not rely on any downscaling principle and (2) a novel method to measure the impact on the biosphere integrity Earth system. Our bottom-up approach quantifies the impact of a technological alternative on the control variables of the PBs by computing a PB transgression metric. This aggregated metric is complemented by an analysis of the (disaggregated) shares of the SOS occupied by each scenario, which sheds light on whether they can pose threats to specific Earth systems.

The PB framework[28] provides both a theoretical and a methodological basis to carry out absolute sustainability assessments considering the carrying capacity of Earth. In 2009, Rockström et al.[27] identified nine key Earth-system processes covering physical, chemical, and biological processes and established a set of PBs on specific control variables defined for them. All the PBs jointly establish the so-called SOS for humanity. The SOS corresponds to the difference between the boundary and the natural background level, which provides the budget for maximum anthropogenic perturbation without compromising the stability and resilience of the Earth system. The authors claim that surpassing these boundaries could trigger a chain of irreversible events at the planetary level, which would threaten our future well-being. In 2015, Steffen et al.[28] updated the framework with a more in-depth analysis of the PBs.

Planetary limits were defined on climate change, stratospheric ozone depletion, ocean acidification, biogeochemical flows of nitrogen and phosphorus, land-system change, freshwater use, biosphere integrity, atmospheric aerosol loading, and introduction of novel entities. The last two Earth-system processes are yet to be adequately quantified and, therefore, were omitted in our analysis. Among the ones considered in our work, climate change and biosphere integrity are of critical importance, as they are regarded as core PBs through which the other boundaries operate.[28] Nevertheless, all of the Earth-system processes and their interactions define the stability of our planet.

The increased interest in the finite capacity of the planet has recently led to novel LCA methods that can underpin absolute environmental sustainability assessments.[26] Notably, Ryberg et al.[33] recently proposed an approach to link emissions and resource consumption to Earth-system processes, thereby enabling the quantification of the performance of a system in terms of the PBs. Our bottom-up methodology, which follows the four LCA steps,[84] applies the characterization models developed by Ryberg et al.[33] (except for the change in biosphere integrity PB, explained later) to quantify the impact on the control variables of the PBs. It next uses these impacts to compute an aggregated PB transgression metric, as discussed below.

In summary, all the LCI elementary flows connected to the PBs (e.g., kg of CO_2 emissions or m^3 of water consumed) are translated into the PB control variables with the use of characterization factors. Considering the set B of PBs b, the environmental burden for each scenario s ($EB_{b,s}$) is quantified with Equation 4:

$$EB_{b,s} = \sum_{c \in C} \sum_{e \in E} LCI_{c,e,s} \cdot CF_{b,e} \cdot PV_c \quad \forall b \in B, s \in S, \qquad \text{(Equation 4)}$$

where $LCI_{c,e,s}$ is the unitary LCI elementary flow e for chemical c in scenario s (where index s denotes the members of the set S); recall that this variable is calculated from Equation 1. $CF_{b,e}$ is the characterization factor for the LCI elementary flow e linked to PB b taken from Ryberg et al.[33] for all the PBs except for the biosphere integrity, for which we apply Equations 5 and 6. PV_c denotes the production volumes of each chemical c based on the expected production for 2020.[4]

We introduce a method to quantify the impact on the biosphere integrity PB, omitted in Ryberg's method,[33] that builds on the work by Hanafiah et al.[34] The latter contribution quantifies the mean species abundance loss caused by the two main stressors of biodiversity loss, i.e., direct land use and CO_2 emissions.[85] These two stressors provide a lower bound on the loss in mean species abundance (MSA, relative to a reference point, i.e., pre-industrial species abundance). We focus on the functional diversity of species PB (which we measured via the MSA) linked to the biosphere integrity Earth system, as defined by Steffen et al.[28] We apply the threshold defined on the Biodiversity Intactness Index (BII) (10% with an uncertainty range 10%–70%), proposed as an interim control variable,[28] to the MSA, regarded as a good proxy of the BII[86] (see assumptions and limitations in Note S3). Considering subset *LU* of land-use types and subset *EM* of GHG emissions, both belonging to set *E* of LCI elementary flows, the characterization factors for direct land use and CO_2 emissions are calculated according to Equations 5 and 6 as follows:

$$CF_{b,e} = \frac{\left(1 - MSA_{b,e}^{LU}\right)}{A^{BL}} \quad \forall b = \text{biosphere integrity}, e \in LU \qquad \text{(Equation 5)}$$

$$CF_{b,e} = \frac{GWP_e^{ReCiPe} \cdot TF_{CO_2} \cdot \left(\sum_k \left(A_k^{BIO} \cdot \left(1 - MSA_{b,k}^{CO_2}\right)\right)\right)}{A^{BL}} \quad \forall b = \text{biosphere integrity}, e \in EM, \qquad \text{(Equation 6)}$$

where $\left(1 - MSA_{b,e}^{LU}\right)$ and $TF_{CO_2} \cdot \left(\sum_k \left(A_k^{BIO} \cdot \left(1 - MSA_{b,k}^{CO_2}\right)\right)\right)$ are the factors provided by Hanafiah et al.[34] for the direct land use and CO_2 emissions stressors, respectively.

The factor for direct land use ($\left(1 - MSA_{b,e}^{LU}\right)$, dimensionless) represents the mean species abundance loss for different land-use types following the Ecoinvent classification;[61] where $MSA_{b,e}^{LU}$ is the biodiversity indicator denoting the mean species abundance for each land use type e. The factor for the CO_2 emissions represents the loss in mean species abundance across biomes k per unit of mass of equivalent CO_2 emissions. The latter factor is determined in two steps; first, the change in the global mean temperature due to a change in carbon emissions is modeled via parameter TF_{CO_2} (°C year kg^{-1}). The temperature change is then translated into abundance loss across biomes with the factor $\sum_k \left(A_k^{BIO} \cdot \left(1 - MSA_{b,k}^{CO_2}\right)\right)$, which is aggregated globally considering a set K of biomes k and their corresponding areas A_k^{BIO}. The characterization factor of the CO_2 emissions, therefore, expresses the abundance loss in natural biomes as a linear function of a steady flow of CO_2; in our case we assume a 100-year time horizon (i.e., 0.27 m^2 year kg^{-1}). Moreover, in Equation 6, GWP_e^{ReCiPe} corresponds to the global warming potential factor for all GHG emissions as provided in ReCiPe 2016[71] for a 100-year time horizon (kg CO_2-eq kg^{-1} GHG), which allows converting any GHG to the equivalent amount of CO_2. Finally, A^{BL} is the total area of the natural and non-natural biomes in the IMAGE model[86] (i.e., $1.3 \cdot 10^{14}$ m^2), which is taken as reference area (undisturbed by human activities). The estimated characterization factors for the biosphere integrity PB by land-use type and for the CO_2 emissions considering different horizons can be found in Table S14 in Galán-Martín et al.[60]

Finally, with the impact on the control variables of the PBs at hand, we quantify a PB transgression metric. This metric simulates the effects on the nine PBs of replacing the fossil-based chemicals (subset BAU = {*Fossil*}), by an alternative scenario (assuming *ceteris paribus* conditions, i.e., all the other sectors would remain unaltered). To this end, we first quantify the global anthropogenic impact that would emerge in every alternative scenario as follows, in Equation 7:

$$EB_{b,s}^{GLO} = EB_b^{CUR} - EB_{b,s'} + EB_{b,s} \quad \forall b \in B, s \in S, s' \in BAU, \qquad \text{(Equation 7)}$$

where $EB_{b,s}^{GLO}$ provides the global anthropogenic environmental impact on each PB b for each scenario s, whereas EB_b^{CUR} corresponds to the current anthropogenic impact level in each PB b (after subtracting the natural background level), as provided by Steffen et al.[28] (except for the biosphere integrity PB, only available for the southern Africa region). The current value of the control variable for the biosphere integrity PB was estimated from Katia et al.[87,88] using ESRI ArcGIS version 10.7.1.[89] We derived a global BII of 73.2% from the abundance-based BII maps as the average across all cells after re-projecting to a Behrmann equal-area projection. This value falls, therefore, below the proposed PB of 90% defined for BII.[28] Moreover, for consistency across PBs, the current impact levels in the climate change and ocean acidification PBs were adjusted according to emissions data in 2015 extracted from EORA.[90] Hence, to ensure a meaningful analysis, we consider the impact on these PBs that would result from keeping the annual flow of emissions steady until 2300, the year taken as a reference to derive the characterization factors in Ryberg et al.[33]

We finally quantify the PB footprint (PBF_s) from the simulated transgression levels in each PB b by comparing the global (predicted) anthropogenic environmental impact ($EB_{b,s}^{GLO}$) with the SOS as defined by Rockström et al.[27] and later updated by Steffen et al.[28] The PB footprint for scenario s (PBF_s) is provided by Equations 8 and 9 as follows:

$$LT_{b,s}^{GLO} = \begin{cases} 0 \text{ if } \dfrac{EB_{b,s}^{GLO}}{SOS_b} < 1 \\ \dfrac{EB_{b,s}^{GLO}}{SOS_b} \text{ otherwise} \end{cases} \quad \forall b \in B, s \in S \qquad \text{(Equation 8)}$$

$$PBF_s = \frac{\sum_b LT_{b,s}^{GLO}}{|B|} \quad \forall s \in S, \qquad \text{(Equation 9)}$$

where the global level of transgression ($LT_{b,s}^{GLO}$) is given by the quotient between the global anthropogenic impact $EB_{b,s}^{GLO}$ and the SOS for each PB b (SOS_b). Note that if the PB is not exceeded, the transgression level is zero. In Equation 9, $|B|$ corresponds to the cardinality of the set B of PBs, i.e., the number of elements in the set B. Here, we could consider different weighting schemes to penalize the transgression levels depending on the current transgression level (yellow or red zones) as well as the PBs (core or non-core). Moreover, we could consider only one PB for the climate change Earth-system process given that both PBs, i.e., energy balance and CO_2 concentration, are mostly driven by CO_2 emissions (see Note S3 on methodological assumptions, limitations, and future work). Without loss of generality, we include the nine PBs and assume here equal weights regardless of the transgression level, i.e., all PBs are equally important.

As an example of how the PB footprint is calculated, the *DAC CCU + BECCS* scenario would lead to new transgression levels of 4.06%, 3.65%, 0.49%, 1.16%, 2.70%, 2.11%, 1.52%, 0.65%, and 3.99% in the climate change energy imbalance, climate change CO_2 concentration, stratospheric ozone depletion, ocean acidification, nitrogen flow, phosphorus flow, land-system change, freshwater use and biosphere integrity PBs, respectively. Hence, the PB footprint of this scenario would be given by the summation of the new transgression levels in the exceeded PBs (all except the stratospheric ozone depletion and freshwater use PBs) divided by the total number of PBs, i.e., nine, that is, 19.20/9 = 2.13. Note that this PB metric is complemented by the analysis of the shares of the SOS occupied by each scenario in the Earth systems, which should be kept as low as possible.

Uncertainty/sensitivity analysis

The LCI data retrieved from Ecoinvent v3.5[61] are affected by numerous uncertainties.[91] The accuracy of our results and robustness of our conclusions under uncertainties in the inventory data (other uncertainties were omitted due to lack of statistical data) were assessed using the Monte Carlo sampling method implemented in Simapro v9.0.[70] Accordingly, we ran 1,000 scenarios from the underlying probability functions that model the LCI elementary flows, as defined in Ecoinvent v3.5. The uncertainty results are illustrated in Figures 2, 4, and 5 by means of boxplots with whiskers following the 1.5 interquartile rule. Further discussion on the uncertainties is included in Note S3 on methodological assumptions, limitations, and future work.

Similarly, a sensitivity analysis was performed on the economic assessment of the six representative scenarios by varying the costs of raw materials and utilities, i.e., cost of biomass, CO_2, H_2, electricity from wind, solar PV, BECCS, and the grid, and the heating needs. To this end, two scenarios were defined, i.e., pessimistic and optimistic, corresponding to the maximum and minimum cost values, respectively. The uncertainty range for the costs is depicted with error bars in Figures 6 and S9.

For the costs of H_2, we considered the low, central, and high estimates provided by Parkinson et al.[51] Due to data gaps, the costs of the electrolytic H_2 from BECCS was estimated with a discounted cash flow analysis (see details on data used in Galán-Martín et al.[60]). For the sensitivity parameters, we consider ranges for the levelized costs of electricity and the CAPEX of the electrolyzer (i.e., ±30% of 0.157 USD_{2015} kWh^{-1}[92] and 800 (400–1,000) USD_{2015} kW^{-1}[51]). For the *BTM* scenario, the cost ranges for the biomass straw and the CAPEX term were sourced from Yang et al.[73] For the cost prospects of H_2, nominal, pessimistic, and optimistic estimates were sourced from the report by the Hydrogen Council.[41] The cost of the CO_2 from natural gas power plants was sourced from Rubin et al.[93] The cost range of CO_2 from DAC was taken from Keith et al.[67] For wind electricity, we defined minimum and maximum levelized costs based on the US Energy Information Administration.[94] For the *Fossil* scenario, nominal prices of olefins and aromatics were sourced from the Petrochemicals Price Assessments Catalog from Platts,[95] whereas maximum and minimum values were derived assuming given annual variations (as reported therein). The range for the methanol price was sourced from the Methanex Corporation.[96] Tables S11 and S12 in Galán-Martín et al.[60] summarize all these cost intervals for the scenarios.

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at https://doi.org/10.1016/j.oneear.2021.04.001.

ACKNOWLEDGMENTS

All authors thank Mark A.J. Huijbregts for his assistance in the development of the biosphere integrity method. This publication was created as part of NCCR Catalysis, a National Centre of Competence in Research funded by the Swiss National Science Foundation.

AUTHOR CONTRIBUTIONS

Conceptualization, A.G.M., V.T., J.P.R., and G.G.G.; methodology, A.G.M. and V.T.; investigation, A.G.M. and V.T.; writing – original draft, A.G.M., V.T., and G.G.G.; writing – review & dditing, A.G.M., V.T., I.D., C.P., J.P.R., and G.G.G.; funding acquisition, J.P.R. and G.G.G.; visualization, A.G.M. and V.T.; supervision, G.G.G.

DECLARATION OF INTERESTS

The authors declare no competing interests.

Received: August 27, 2020
Revised: November 26, 2020
Accepted: April 1, 2021
Published: April 23, 2021

REFERENCES

1. IPCC (2018). Global Warming of 1.5°C: An IPCC Special Report on the Impacts of Global Warming of 1.5°C above Pre-industrial Levels and Related Global Greenhouse Gas Emission Pathways, in the Context of Strengthening the Global Response to the Threat of Climate Change. https://www.ipcc.ch/sr15/.
2. IEA, ICCA, and DECHEMA (2013). Technology Roadmap Energy and GHG Reductions in the Chemical Industry via Catalytic Processes. https://www.iea.org/reports/technology-roadmap-energy-and-ghg-reductions-in-the-chemical-industry-via-catalytic-processes.
3. Schiffer, Z.J., and Manthiram, K. (2017). Electrification and decarbonization of the chemical industry. Joule *1*, 10–14.
4. Bazzanella, A.M., and Ausfelder, F. (2017). Low carbon energy and feedstock for the European chemical industry. https://dechema.de/en/Low_carbon_chemical_industry-path-123212,124930.html.
5. Kätelhön, A., Meys, R., Deutz, S., Suh, S., and Bardow, A. (2019). Climate change mitigation potential of carbon capture and utilization in the chemical industry. Proc. Natl. Acad. Sci. USA *116*, 11187–11194.
6. Boulamanti, A., and Moya, J.A. (2017). Energy efficiency and GHG emissions: Prospective scenarios for the Chemical and Petrochemical Industry. https://ec.europa.eu/jrc/en/publication/eur-scientific-and-technical-research-reports/energy-efficiency-and-ghg-emissions-prospective-scenarios-chemical-and-petrochemical.
7. Gabrielli, P., Gazzani, M., and Mazzotti, M. (2020). The Role of Carbon Capture and Utilization, Carbon Capture and Storage, and Biomass to Enable a Net-Zero-CO_2 Emissions Chemical Industry. Ind. Eng. Chem. Res. *59*, 7033–7045.
8. Hepburn, C., Adlen, E., Beddington, J., Carter, E.A., Fuss, S., Mac Dowell, N., Minx, J.C., Smith, P., and Williams, C.K. (2019). The technological and economic prospects for CO_2 utilization and removal. Nature *575*, 87–97.
9. Majumdar, A., and Deutch, J. (2018). Research opportunities for CO_2 utilization and negative emissions at the Gigatonne Scale. Joule *2*, 805–809.
10. Al-Qahtani, A., González-Garay, A., Bernardi, A., Galán-Martín, Á., Pozo, C., Mac Dowell, N., Chachuat, B., and Guillén-Gosálbez, G. (2020). Electricity grid decarbonisation or green methanol fuel? A life-cycle modelling and analysis of today's transportation-power nexus. Appl. Energy *265*, 114718.
11. González-Garay, A., Frei, M.S., Al-Qahtani, A., Mondelli, C., Guillén-Gosálbez, G., and Pérez-Ramírez, J. (2019). Plant-to-planet analysis of CO_2-based methanol processes. Energy Environ. Sci. *12*, 3425–3436.
12. Cuéllar-Franca, R.M., and Azapagic, A. (2015). Carbon capture, storage and utilisation technologies: A critical analysis and comparison of their life cycle environmental impacts. J. CO2 Util. *9*, 82–102.
13. Boot-Handford, M.E., Abanades, J.C., Anthony, E.J., Blunt, M.J., Brandani, S., Mac Dowell, N., Fernández, J.R., Ferrari, M.-C., Gross, R., and Hallett, J.P. (2014). Carbon capture and storage update. Energy Environ. Sci. *7*, 130–189.
14. Styring, P., Quadrelli, E.A., and Armstrong, K. (2014). Carbon dioxide utilisation: closing the carbon cycle (Elsevier).
15. Otto, A., Grube, T., Schiebahn, S., and Stolten, D. (2015). Closing the loop: Captured CO_2 as a feedstock in the chemical industry. Energy Environ. Sci. *8*, 3283–3297.
16. Al-Mamoori, A., Krishnamurthy, A., Rownaghi, A.A., and Rezaei, F. (2017). Carbon capture and utilization update. Energy Technol. *5*, 834–849.
17. de Jong, E., Higson, A., Walsh, P., and Wellisch, M. (2012). Bio-based chemicals value added products from biorefineries. https://www.ieabioenergy.com/blog/publications/bio-based-chemicals-value-added-products-from-biorefineries/.
18. Wesseling, J.H., Lechtenböhmer, S., Åhman, M., Nilsson, L.J., Worrell, E., and Coenen, L. (2017). The transition of energy intensive processing industries towards deep decarbonization: Characteristics and implications for future research. Renew. Sustain. Energy Rev. *79*, 1303–1313.
19. Sachs, J.D., Schmidt-Traub, G., Mazzucato, M., Messner, D., Nakicenovic, N., and Rockström, J. (2019). Six Transformations to achieve the Sustainable Development Goals. Nat. Sustain. *2*, 805–814.
20. IEA (2017). Energy Technology Perspectives 2017 - Catalysing Energy Technology Transformations (OECD).
21. Pérez-Fortes, M., Schöneberger, J.C., Boulamanti, A., and Tzimas, E. (2016). Methanol synthesis using captured CO_2 as raw material: Techno-economic and environmental assessment. Appl. Energy *161*, 718–732.
22. Sternberg, A., Jens, C.M., and Bardow, A. (2017). Life cycle assessment of CO_2-based C1-chemicals. Green Chem. *19*, 2244–2259.

23. Mac Dowell, N., Fennell, P.S., Shah, N., and Maitland, G.C. (2017). The role of CO_2 capture and utilization in mitigating climate change. Nat. Clim. Chang. *7*, 243–249.

24. Meunier, N., Chauvy, R., Mouhoubi, S., Thomas, D., and De Weireld, G. (2020). Alternative production of methanol from industrial CO_2. Renew. Energy *146*, 1192–1203.

25. Thonemann, M.A.N. (2020). Environmental impacts of CO_2-based chemical production: A systematic literature review and meta-analysis. Appl. Energy *263*, 114599.

26. Bjørn, A., Chandrakumar, C., Boulay, A.-M., Doka, G., Fang, K., Gondran, N., Hauschild, M.Z., Kerkhof, A., King, H., Margni, M., et al. (2020). Review of life-cycle based methods for absolute environmental sustainability assessment and their applications. Environ. Res. Lett. *15*, 083001.

27. Rockström, J., Steffen, W., Noone, K., Persson, A., Chapin, F.S., 3rd, Lambin, E.F., Lenton, T.M., Scheffer, M., Folke, C., Schellnhuber, H.J., et al. (2009). A safe operating space for humanity. Nature *461*, 472–475.

28. Steffen, W., Richardson, K., Rockström, J., Cornell, S.E., Fetzer, I., Bennett, E.M., Biggs, R., Carpenter, S.R., de Vries, W., de Wit, C.A., et al. (2015). Sustainability. Planetary boundaries: guiding human development on a changing planet. Science *347*, 1259855.

29. O'Neill, D.W., Fanning, A.L., Lamb, W.F., and Steinberger, J.K. (2018). A good life for all within planetary boundaries. Nat. Sustain. *1*, 88–95.

30. Lade, S.J., Steffen, W., de Vries, W., Carpenter, S.R., Donges, J.F., Gerten, D., Hoff, H., Newbold, T., Richardson, K., and Rockström, J. (2019). Human impacts on planetary boundaries amplified by Earth system interactions. Nat. Sustain. 1–10.

31. Verburg, P.H., Dearing, J.A., Dyke, J.G., Van Der Leeuw, S., Seitzinger, S., Steffen, W., and Syvitski, J. (2016). Methods and approaches to modelling the Anthropocene. Glob. Environ. Change *39*, 328–340.

32. Sterner, T., Barbier, E.B., Bateman, I., van den Bijgaart, I., Crépin, A.-S., Edenhofer, O., Fischer, C., Habla, W., Hassler, J., and Johansson-Stenman, O. (2019). Policy design for the Anthropocene. Nat. Sustain. *2*, 14.

33. Ryberg, M.W., Owsianiak, M., Richardson, K., and Hauschild, M.Z. (2018). Development of a life-cycle impact assessment methodology linked to the Planetary Boundaries framework. Ecol. Indic. *88*, 250–262.

34. Hanafiah, M.M., Hendriks, A.J., and Huijbregts, M.A.J. (2012). Comparing the ecological footprint with the biodiversity footprint of products. J. Clean. Prod. *37*, 107–114.

35. von der Assen, N., Voll, P., Peters, M., and Bardow, A. (2014). Life cycle assessment of CO_2 capture and utilization: a tutorial review. Chem. Soc. Rev. *43*, 7982–7994.

36. Levi, P.G., and Cullen, J.M. (2018). Mapping global flows of chemicals: from fossil fuel feedstocks to chemical products. Environ. Sci. Technol. *52*, 1725–1734.

37. Oxford Economics (2019). The Global Chemical Industry: Catalyzing Growth and Addressing Our World's Sustainability Challenges. https://www.oxfordeconomics.com/recent-releases/the-global-chemical-industry-catalyzing-growth-and-addressing-our-world-sustainability-challenges.

38. Lucas, P.L., Wilting, H.C., Hof, A.F., and van Vuuren, D.P. (2020). Allocating planetary boundaries to large economies: Distributional consequences of alternative perspectives on distributive fairness. Glob. Environ. Change *60*, 102017.

39. Huijbregts, M.A.J., Rombouts, L.J.A., Hellweg, S., Frischknecht, R., Hendriks, A.J., Van de Meent, D., Ragas, A.M.J., Reijnders, L., and Struijs, J. (2006). Is cumulative fossil energy demand a useful indicator for the environmental performance of products? Environ. Sci. Technol. *40*, 641–648.

40. IEA (2019). World Energy Outlook 2019. https://www.iea.org/reports/world-energy-outlook-2019.

41. Hydrogen Council (2020). Path to hydrogen competitiveness: A cost perspective. https://hydrogencouncil.com/en/path-to-hydrogen-competitiveness-a-cost-perspective/.

42. IEA (2018). Global Energy & CO_2 Status Report 2018. https://webstore.iea.org/global-energy-co2-status-report-2018.

43. Chum, H., Faaij, A., Moreira, J., Berndes, G., Dhamija, P., Dong, H., Gabrielle, B., Goss Eng, A., Lucht, W., Mapako, M., et al. (2011). Bioenergy. In IPCC Special Report on Renewable Energy Sources and Climate Change Mitigation, O. Edenhofer, R. Pichs-Madruga, Y. Sokona, K. Seyboth, P. Matschoss, S. Kadner, T. Zwickel, P. Eickemeier, G. Hansen, S. Schlömer, and C. von Stechow, eds. (Cambridge University Press), pp. 209–332.

44. Daioglou, V., Stehfest, E., Wicke, B., Faaij, A., and van Vuuren, D.P. (2016). Projections of the availability and cost of residues from agriculture and forestry. Glob. Change Biol. Bioenergy *8*, 456–470.

45. Fuss, S., Lamb, W.F., Callaghan, M.W., Hilaire, J., Creutzig, F., Amann, T., Beringer, T., de Oliveira Garcia, W., Hartmann, J., and Khanna, T. (2018). Negative emissions-Part 2: Costs, potentials and side effects. Environ. Res. Lett. *13*, 63002.

46. Dooley, J.J. (2013). Estimating the supply and demand for deep geologic CO_2 storage capacity over the course of the 21st century: A meta-analysis of the literature. In Energy Procedia (Elsevier), pp. 5141–5150.

47. IEA (2018). World Energy Balances 2018 (IEA).

48. Heck, V., Gerten, D., Lucht, W., and Popp, A. (2018). Biomass-based negative emissions difficult to reconcile with planetary boundaries. Nat. Clim. Chang. *8*, 151–155.

49. Gleeson, T., Wang-Erlandsson, L., Zipper, S.C., Porkka, M., Jaramillo, F., Gerten, D., Fetzer, I., Cornell, S.E., Piemontese, L., and Gordon, L.J. (2020). The water planetary boundary: interrogation and revision. One Earth *2*, 223–234.

50. Staffell, I., Scamman, D., Abad, A.V., Balcombe, P., Dodds, P.E., Ekins, P., Shah, N., and Ward, K.R. (2019). The role of hydrogen and fuel cells in the global energy system. Energy Environ. Sci. *12*, 463–491.

51. Parkinson, B., Balcombe, P., Speirs, J.F., Hawkes, A.D., and Hellgardt, K. (2019). Levelized cost of CO_2 mitigation from hydrogen production routes. Energy Environ. Sci. *12*, 19–40.

52. IRENA (2019). Innovation landscape brief: Renewable Power-to-Hydrogen (International Renewable Energy Agency).

53. Realmonte, G., Drouet, L., Gambhir, A., Glynn, J., Hawkes, A., Köberle, A.C., and Tavoni, M. (2019). An inter-model assessment of the role of direct air capture in deep mitigation pathways. Nat. Commun. *10*, 3277.

54. Pozo, C., Galán-Martín, Á., Reiner, D.M., Mac Dowell, N., and Guillén-Gosálbez, G. (2020). Equity in allocating carbon dioxide removal quotas. Nat. Clim. Chang. *10*, 640–646.

55. European Commission (2020). Proposal for a REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL establishing the framework for achieving climate neutrality and amending Regulation (EU) 2018/1999 (European Climate Law).

56. Häyhä, T., Lucas, P.L., van Vuuren, D.P., Cornell, S.E., and Hoff, H. (2016). From Planetary Boundaries to national fair shares of the global safe operating space — How can the scales be bridged? Glob. Environ. Change *40*, 60–72.

57. European Union (2013). Environmental Taxes - A Statistical Guide - 2013 edition. https://ec.europa.eu/eurostat/web/products-manuals-and-guidelines/-/KS-GQ-13-005.

58. Bjørn, A., Sim, S., King, H., Margni, M., Henderson, A.D., Payen, S., and Bulle, C. (2020). A comprehensive planetary boundary-based method for the nitrogen cycle in life cycle assessment: Development and application to a tomato production case study. Sci. Total Environ. *715*, 136813.

59. Bjørn, A., Sim, S., King, H., Patouillard, L., Margni, M., Hauschild, M.Z., and Ryberg, M. (2020). Life cycle assessment applying planetary and regional boundaries to the process level: a model case study. Int. J. Life Cycle Assess. *25*, 2241–2254.

60. Galán-Martín, Á., Tulus, V., Díaz, I., Pozo, C., Pérez-Ramírez, J., and Guillén-Gosálbez, G. (2021). Dataset: Sustainability footprints of a renewable carbon transition for the chemical sector within planetary boundaries (Zenodo). https://doi.org/10.5519/0000082.

61. Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., and Weidema, B. (2016). The ecoinvent database version 3 (part I): overview and methodology. Int. J. Life Cycle Assess. *21*, 1218–1230.

62. Liu, Y., Li, G., Chen, Z., Shen, Y., Zhang, H., Wang, S., Qi, J., Zhu, Z., Wang, Y., and Gao, J. (2020). Comprehensive analysis of environmental impacts and energy consumption of biomass-to-methanol and coal-to-methanol via life cycle assessment. Energy *204*, 117961.

63. Dufour, J., Serrano, D.P., Gálvez, J.L., González, A., Soria, E., and Fierro, J.L.G. (2012). Life cycle assessment of alternatives for hydrogen production from renewable and fossil sources. Int. J. Hydrogen Energy *37*, 1173–1183.

64. Susmozas, A., Iribarren, D., Zapp, P., Linben, J., and Dufour, J. (2016). Life-cycle performance of hydrogen production via indirect biomass gasification with CO_2 capture. Int. J. Hydrogen Energy *41*, 19484–19491.

65. Iribarren, D., Petrakopoulou, F., and Dufour, J. (2013). Environmental and thermodynamic evaluation of CO_2 capture, transport and storage with and without enhanced resource recovery. Energy *50*, 477–485.

66. Petrakopoulou, F., Iribarren, D., and Dufour, J. (2015). Life-cycle performance of natural gas power plants with pre-combustion CO_2 capture. Greenh. Gases Sci. Technol. *5*, 268–276.

67. Keith, D.W., Holmes, G., St. Angelo, D., and Heidel, K. (2018). A Process for Capturing CO_2 from the Atmosphere. Joule *2*, 1573–1594.

68. ISO 14040:2006(E). (2016). Environmental management — Life cycle assessment — Principles and framework.

69. ISO 14044:2006(E). (2016). Environmental management — Life cycle assessment — Requirements and guidelines.

70. Goedkoop, M., Oele, M., Leijting, J., Ponsioen, T., and Meijer, E. (2016). Introduction to LCA with SimaPro. https://pre-sustainability.com/files/2014/05/SimaPro8IntroductionToLCA.pdf.

71. Huijbregts, M.A.J., Steinmann, Z.J.N., Elshout, P.M.F., Stam, G., Verones, F., Vieira, M.D.M., Hollander, A., Zijp, M., and van Zelm, R. (2017). ReCiPe 2016: A harmonized life cycle impact assessment method at midpoint and endpoint level Report I: Characterization. The International Journal of Life Cycle Assessment *22*, 138–147.

72. Spallina, V., Velarde, I.C., Jimenez, J.A.M., Godini, H.R., Gallucci, F., and Van Sint Annaland, M. (2017). Techno-economic assessment of different routes for olefins production through the oxidative coupling of methane (OCM): Advances in benchmark technologies. Energy Convers. Manage. *154*, 244–261.

73. Yang, S., Li, B., Zheng, J., and Kankala, R.K. (2018). Biomass-to-Methanol by dual-stage entrained flow gasification: Design and techno-economic analysis based on system modeling. J. Clean. Prod. *205*, 364–374.

74. Gasol, C.M., Gabarrell, X., Anton, A., Rigola, M., Carrasco, J., Ciria, P., and Rieradevall, J. (2009). LCA of poplar bioenergy system compared with Brassica carinata energy crop and natural gas in regional scenario. Biomass Bioenergy *33*, 119–129.

75. Lee, J., An, S., Cha, K., and Hur, T. (2010). Life cycle environmental and economic analyses of a hydrogen station with wind energy. Int. J. Hydrogen Energy *35*, 2213–2225.

76. Van Leeuwen Charlotte, Z.A. (2018). Innovative large-scale energy storage technologies and Power-to-Gas concepts after optimisation. D8.3–Report on the costs involved with PtG technologies and their potentials across the EU. https://cordis.europa.eu/project/id/691797.

77. Aspentech (2016). Aspen HYSYS V9.0.

78. Dutta, A., Karimi, I.A., and Farooq, S. (2019). Technoeconomic Perspective on Natural Gas Liquids and Methanol as Potential Feedstocks for Producing Olefins. Ind. Eng. Chem. Res. *58*, 963–972.

79. Luyben, W.L. (2017). Estimating refrigeration costs at cryogenic temperatures. Comput. Chem. Eng. *103*, 144–150.

80. Zhang, D., Yang, M., and Feng, X. (2019). Aromatics production from methanol and pentane: Conceptual process design, comparative energy and techno-economic analysis. Comput. Chem. Eng. *126*, 178–188.

81. Müller, L.J., Kätelhön, A., Bringezu, S., McCoy, S., Suh, S., Edwards, R., Sick, V., Kaiser, S., Cuéllar-Franca, R., El Khamlichi, A., et al. (2020). The carbon footprint of the carbon feedstock CO_2. Energy Environ. Sci. *13*, 2979–2992.

82. Guinée, J.B., Heijungs, R., and Huppes, G. (2004). Economic Allocation: Examples and Derived Decision Tree. Int. J. Life Cycle Assess. *9*, 23–33.

83. von der Assen, N., Jung, J., and Bardow, A. (2013). Life-cycle assessment of carbon dioxide capture and utilization: Avoiding the pitfalls. Energy Environ. Sci. *6*, 2721–2734.

84. Finkbeiner, M., Inaba, A., Tan, R.B.H., Christiansen, K., and Klüppel, H.J. (2006). The new international standards for life cycle assessment: ISO 14040 and ISO 14044. Int. J. Life Cycle Assess. *11*, 80–85.

85. Baisero, D., Visconti, P., Pacifici, M., Cimatti, M., and Rondinini, C. (2020). Projected Global Loss of Mammal Habitat Due to Land-Use and Climate Change. One Earth *2*, 578–585.

86. Alkemade, R., Van Oorschot, M., Miles, L., Nellemann, C., Bakkenes, M., and Ten Brink, B. (2009). GLOBIO3: A framework to investigate options for reducing global terrestrial biodiversity loss. Ecosystems (N. Y.) *12*, 374–390.

87. Newbold, T., Hudson, L.N., Arnell, A.P., Contu, S., De Palma, A., Ferrier, S., Hill, S.L.L., Hoskins, A.J., Lysenko, I., Phillips, H.R.P., et al. (2016). Has land use pushed terrestrial biodiversity beyond the planetary boundary? A global assessment. Science *353*, 288–291.

88. Sanchez-Ortiz, K., Newbold, T., Purvis, A., and de Palma, A. (2019). Dataset: Global maps of Biodiversity Intactness Index (Sanchez-Ortiz et al., 2019 - bioRxiv) (Natural History Museum Data Portal). https://doi.org/10.5519/0000082.

89. Esri (2019). ArcGIS 10.7.1.

90. Lenzen, M., Moran, D., Kanemoto, K., and Geschke, A. (2013). Building Eora: a global multi-region input–output database at high country and sector resolution. Econ. Syst. Res. *25*, 20–49.

91. Huijbregts, M.A.J., Norris, G., Bretz, R., Ciroth, A., Maurice, B., von Bahr, B., Weidema, B., and de Beaufort, A.S.H. (2001). Framework for modelling data uncertainty in life cycle inventories. Int. J. Life Cycle Assess. *6*, 127.

92. Cabral, R.P., Bui, M., and Mac Dowell, N. (2019). A synergistic approach for the simultaneous decarbonisation of power and industry via bioenergy with carbon capture and storage (BECCS). Int. J. Greenh. Gas Control *87*, 221–237.

93. Rubin, E.S., Davison, J.E., and Herzog, H.J. (2015). The cost of CO_2 capture and storage. Int. J. Greenh. Gas Control *40*, 378–400.

94. US Energy Information Administration (2019). Levelized cost and levelized avoided cost of new generation resources in the Annual Energy Outlook 2019. https://www.eia.gov/outlooks/archive/aeo19/pdf/electricity_generation.pdf.

95. S&P Global Platts. Petrochemicals price assessments catalog. https://www.spglobal.com/platts/en/our-methodology/price-assessments/petrochemicals.

96. Methanex. Methanol prices for North America, Europe and Asia. https://www.methanex.com/our-business/pricing.