CellPress
OPEN ACCESS

One Earth

Review

# Net-zero emissions chemical industry in a world of limited resources

**Paolo Gabrielli,[1,2,*] Lorenzo Rosa,[2] Matteo Gazzani,[3,4] Raoul Meys,[5] André Bardow,[1] Marco Mazzotti,[1] and Giovanni Sansavini[1]**
[1]Institute of Energy and Process Engineering, ETH Zurich, 8092 Zurich, Switzerland
[2]Department of Global Ecology, Carnegie Institution for Science, Stanford, CA 94305, USA
[3]Utrecht University, Copernicus Institute of Sustainable Development, Princetonlaan 8a, 3584 CB Utrecht, the Netherlands
[4]Sustainable Process Engineering, Chemical Engineering and Chemistry, Eindhoven University of Technology, 5612 AP Eindhoven, the Netherlands
[5]Carbon Minds GmbH, 50933 Cologne, Germany
*Correspondence: gapaolo@ethz.ch

https://doi.org/10.1016/j.oneear.2023.05.006

## SUMMARY

**The chemical industry is responsible for about 5% of global $CO_2$ emissions and is key to achieving net-zero targets. Decarbonizing this industry, nevertheless, faces particular challenges given the widespread use of carbon-rich raw materials, the need for high-temperature heat, and the complex global value chains. Multiple technology routes are now available for producing chemicals with net-zero $CO_2$ emissions based on biomass, recycling, and carbon capture, utilization, and storage. However, the extent to which these routes are viable with respect to local availability of energy and natural resources remains unclear. In this review, we compare net-zero routes by quantifying their energy, land, and water requirements and the corresponding induced resource scarcity at the country level and further discuss the technical and environmental viability of a net-zero chemical industry. We find that a net-zero chemical industry will require location-specific integrated solutions that combine net-zero routes with circular approaches and demand-side measures and might result in a reshaping of the global chemicals trade.**

## INTRODUCTION

To keep global warming below the 1.5°C threshold stipulated by the Paris Agreement, all anthropogenic $CO_2$ emissions will have to reach net zero by around mid-century, with all greenhouse gas (GHG) emissions achieving net zero soon after.[1,2] In a world of net-zero $CO_2$ emissions (hereafter simply referred to as net-zero) at steady state, any carbon atom extracted from the subsurface will have to be permanently returned to it, lest it is sooner or later emitted to the atmosphere. Any carbon atom released into the atmosphere will have to be pulled back out of it to avoid the rise of carbon concentration in the atmosphere and, hence, the global average temperature.[3]

Some energy services such as electricity, residential heating and cooling, and light-duty transport may be relatively easy to decarbonize by electrifying and generating carbon-free (C-free) electricity. However, electrification is insufficient for so-called hard-to-abate industries, such as the chemical, aviation, cement, iron, and steel industries, responsible for nearly one-third of global carbon emissions.[4] In hard-to-abate industries, carbon emissions are mainly due to the need for high-temperature heat and carbon as a material feedstock, e.g., in chemical products, such as plastics. Thus, achieving net-zero emissions requires combining C-free energy supply with $CO_2$-neutral carbon feedstock.

Within hard-to-abate industries, the chemical industry is vital in climate discussions.[5,6] First, chemical production is very energy- and $CO_2$-intensive. Moreover, chemical products are ubiquitous and integrated across multiple supply chains, with around 96% of all manufactured goods being touched by chemistry.[7,8] Today the chemical industry emits about 2 billion metric tons of $CO_2$ ($GtCO_2$) per year (direct and energy emissions), accounting for about 5% of global GHG emissions.

Furthermore, the chemical industry faces a particular challenge, as most chemical products contain carbon and it is, therefore, virtually impossible to decarbonize. Yet multiple technology routes are available for producing chemicals with net-zero $CO_2$ emissions based on biomass, $CO_2$ use, recycling, and carbon capture and storage. However, all these routes are potentially limited by the local availability of energy and natural resources, such as land and water. Whereas multiple studies assess the viability of a net-zero chemical industry concerning global resources,[9–13] geographical differences are unresolved. Thus, the net-zero chemical industry's technical, environmental, and biophysical viability remains less clear for different countries based on local requirements and resources.

In this review, we examine the feasibility of the technology routes to attain net-zero $CO_2$ emissions in the production of chemicals, accounting for geographical specificities. In the presence of existing knowledge, we assess and compare available

© 2023 The Author(s). Published by Elsevier Inc.
This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

technology routes to achieve net-zero $CO_2$ emissions in the production of all primary chemicals, namely ammonia, methanol, and plastics. The assessment is performed on a country level and coupled with geospatial analysis to determine the land and water scarcity induced by a net-zero chemical industry worldwide. Findings show that a net-zero chemical industry will require integrated solutions that combine net-zero routes with circularity and demand-side measures; such integrated solutions will have to differ regionally based on available resources regarding renewable energy, land, and water availability. Also, our results suggest a potential reshaping of the international trading of chemicals, with the production of chemicals moving from countries with fossil resources to countries with renewable energy, land, and water resources.

## CURRENT STATE OF GLOBAL CHEMICAL INDUSTRY

When counting the biorefineries across the forests and lakes of south-east Finland, it almost feels as if we are on the right track for a post-fossil chemical industry: the pulp and paper industry and the wood industry provide a sustainable carbon-neutral feedstock for the synthesis of many valuable chemicals. One such example is the UPM biorefinery in Lappeenranta, where black liquor waste from pulp and paper manufacture is converted into renewable diesel. This speaks for the ambitious climate goals of the Finnish chemical industry: to be carbon neutral by 2045.[14] However, when looking at global trends in the chemical industry, it is evident that the world is heading in a different direction: the demand for chemicals is rising and so are the associated $CO_2$ emissions[15] (Figure 1).

### Relevance of chemical products and primary chemicals

The demand for chemicals is related to a vast array of products that are produced on the basis of so-called primary chemicals (Box 1). These include methanol, ammonia, and high-value chemicals (ethylene, propylene, benzene, toluene, xylenes), which are the key precursors to plastics.[15] Methanol and high-value chemicals (and plastics) are carbon-based (C-based), while ammonia is C-free. Primary chemicals can either be used directly, e.g., ammonia and methanol as fuels, or to produce other products, e.g., high-value chemicals are mainly used to produce plastics.[20]

Figure 1 provides an overview of the global production and $CO_2$ emissions associated with the primary chemicals in 2020 and 2050. Ammonia is the only primary chemical for which projected $CO_2$ emissions in 2050 are lower than current $CO_2$ emissions, since its production can be decarbonized by electrifying hydrogen production.[17] Plastics production alone is responsible for about 1.4 $GtCO_2$ per year (Figure 1A).[15,27,16] Under business-as-usual (BAU) scenarios where the industry follows current trends, such as the Stated Policies Scenario defined by the International Energy Agency,[28] the emissions related to the chemical industry are projected to be about 4.5 $GtCO_2$ per year in 2050 (Figure 1A).[17,18]

### Challenges of chemical industry toward net zero

As most chemical end-products contain carbon, it is difficult to envision a chemical industry without C-based feedstock and primary chemicals.[7] Thus, in the case of the chemical industry one should not talk about decarbonization but rather focus on how it could achieve net-zero emissions. In fact, the chemical industry uses fossil fuels primarily as raw materials to provide carbon and/or hydrogen to the final products, with about 50% of the energy input to the chemical industry being required as feedstock.[15] While both carbon and hydrogen are largely available in nature, they are constituent parts of more complex molecules, e.g., water, $CO_2$, fossil fuels, and biomass. The chemical industry has historically favored the use of fossil fuels above other abundant molecules, as they embed the energy required for product synthesis rather than requiring it. In many plausible future scenarios, where fossil fuels are phased out from other sectors, the chemical industry is expected to become the largest driver

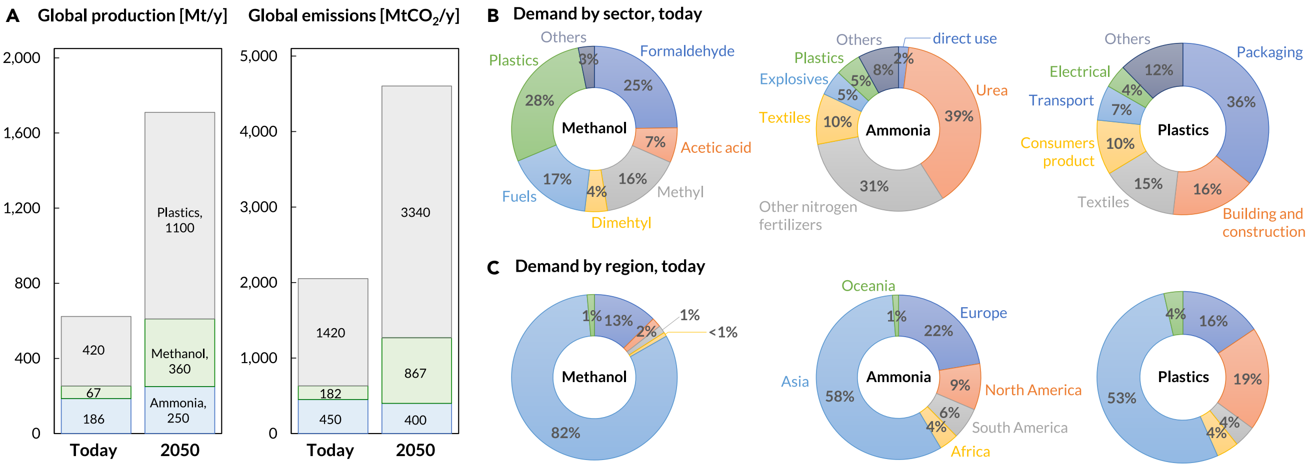

**Figure 1. Global production and $CO_2$ emissions associated with the primary chemicals in 2020 and 2050**

(A) Global production (Mt/year) and $CO_2$ emissions ($MtCO_2$/year) of plastics (gray), methanol (green), and ammonia (blue) for 2020,[15,16] and 2050 values under business-as-usual scenarios.[17,18,19] For both 2020 and 2050, the production of methanol is reported without considering the fraction used to produce plastics.

(B) End-use demand on a mass base of methanol, ammonia, and plastics per market sector.[15,17,18]

(C) End-use demand on a mass base of methanol, ammonia, and plastics per geographical region.[17,16,18].

**Box 1. Primary chemicals**

**METHANOL**

($CH_3OH$). Methanol production is currently the fastest rising of all primary chemicals, with a 21% increase from 2015 to 2020 and a global production of about 91 Mt/year in 2020 (decline from 98 Mt/year in 2019 due to the Covid-19 pandemic).[15] Methanol is mostly used for producing other chemicals such as formaldehyde, which is employed to manufacture several specialized plastics, coatings, and acetic acid. Methanol is also used for fuel applications (the main driver of its above-average demand growth) and as an intermediary to produce high-value chemicals (ethylene, propylene, benzene, toluene, xylenes), hence plastics (Figure 1B).[15,18] Methanol demand and production capacity are highly concentrated in the Asia-Pacific region, due to the rise in petrochemical production in the region. China is the global leader in methanol consumption owing to a sharp rise in the use of methanol in fuel products (Figure 1C).[15]

**AMMONIA**

($NH_3$). Ammonia is the precursor to most nitrogen fertilizers and makes an important contribution to global food security.[21,22] It is estimated that the food provision for half of the world population depends on synthetically produced ammonia fertilizers.[21,22,23] About 70% (131 Mt/year) of ammonia is used to make fertilizers, with the remainder being mostly used to produce plastics, explosives, and synthetic fibers (Figure 1B).[17] With food demand expected to double by 2050, demand for ammonia is expected to increase by 40% (Figure 1B).[17,24] The greatest contribution to ammonia's demand comes from the Asia-pacific region (Figure 1C), due to the large-scale agricultural activities in the region, mostly in India and China.[25]

**PLASTICS**

Demand for plastics drives demand for high-value chemicals, which are the key precursors to most plastics. Between 1950 and 2020, plastics production increased from 2 to 420 Mt/year,[26] with a 12% increase from 2015 to 2020.[15] Plastics production is projected to achieve 1100 Mt/year in 2050, resulting in a carbon footprint (direct and energy $CO_2$ emissions) of about 3.5 $GtCO_2$/year in a BAU scenario (Figure 1). It is worth mentioning that the carbon footprint of plastics is significantly higher than that of high-value chemicals (1.4 $GtCO_2$/year versus 250 $MtCO_2$/year in 2020), due to the high carbon intensity of the processes transforming high-value chemicals into plastics.[16] Major plastic end-use sectors are packaging, building and construction, textiles, and transport applications (Figure 1B). Similar to methanol and ammonia, the greatest contribution to plastics demand comes from the Asia-Pacific region, although Europe and North America play a greater role (Figure 1C).

of global oil consumption by 2050, going from about 10 to 15 million barrels of oil from today to 2050, hence nearly doubling its contribution from 12% today to 25% in 2050.[29,30] However, with more than 60 countries worldwide having pledged to become carbon neutral by 2050,[31,32] the emissions of the chemical sector will need to peak in the next few years and decline around 2030.[15]

## HOW TO ENABLE A NET-ZERO CHEMICAL INDUSTRY

### Available routes for net-zero chemicals production

The chemical industry can continue to deliver its service while complying with net-zero targets through multiple production routes.[33,34] These are illustrated in Figure 2, together with the current BAU route.

#### *Business-as-usual*

A fossil fuel provides the carbon atoms, the hydrogen atoms, and most of the energy required for the product synthesis. Such fossil-based industry yields net-positive $CO_2$ emissions into the atmosphere over the product lifetime, which is typically significantly shorter than any climate-relevant timescale. The bulk $CO_2$ emissions are due to the product synthesis and, for C-based chemicals, to the end-of-life of the carbon content (e.g., via combustion or decomposition). Additional $CO_2$ emissions are due to fossil fuel extraction and preparation, as well as leakages along the supply chain, which can contribute up to about 20% of the total emissions.[16,35]

Within BAU, improvements to efficiency and carbon intensity are underway by reducing the use of coal, recovery of waste heat, electrification (e.g., of steam crackers), and switching from steam boilers to steam/power co-generation.[30] For example, the European chemical industry recorded a 58% reduction in $CO_2$ emissions from 1990 to 2017, despite the growth of the sector.[7] Therefore, further efficiency gains in chemical production are expected to have a relatively modest impact in terms of energy and emissions savings, and more transformative measures will be required.[36]

#### *Carbon capture and storage*

In the carbon capture and storage (CCS) route, chemicals are still synthesized from fossil fuels using the current organic chemistry (the same as BAU). However, all $CO_2$ emissions generated along the chain (i.e., product synthesis, end-of-life, and other $CO_2$-positive processes) are captured and permanently stored in suitable underground geological structures or in building materials. $CO_2$ can be captured exclusively from the air via direct air capture (DAC) or via a combination of point-source capture (PSC) and DAC. PSC is more favorable costs- and energy-wise, but might not always be viable.[37] Overall, CCS routes are available today at a commercial scale, with costs that range from a few tens of US dollars per $tCO_2$ for

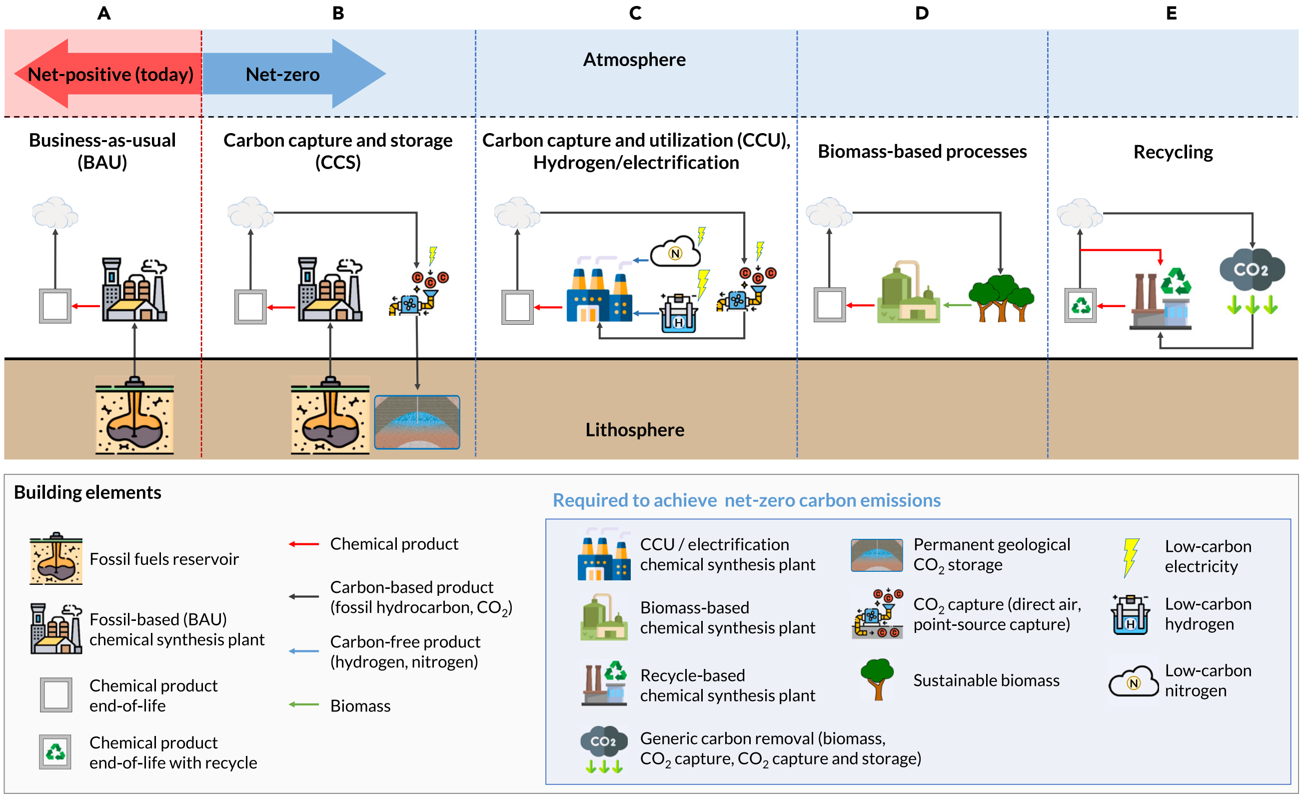

**Figure 2. Available technology routes for net-zero chemical industry**

Schematic representation of the main available routes for the production of chemicals via: (A) business-as-usual (BAU); (B) carbon capture and storage (CCS); (C) carbon capture and utilization (CCU) for carbon-rich chemicals and hydrogen/electrification for carbon-free chemicals; (D) biomass-based synthesis; and (E) carbon recycling. While case (A) is $CO_2$ positive, cases (B), (C), and (D) can all achieve net-zero $CO_2$ emissions, as long as they can rely on carbon-free energy. Carbon recycling, case (E), must be coupled with some sort of carbon removal, i.e., with one of the other net-zero routes, to offset the fraction of chemical products that cannot be recycled, hence to achieve net-zero emissions. All net-zero production routes can be coupled with demand-side strategies to reduce the resources needed to achieve net-zero emissions. Note that: (1) $CO_2$ can be captured via direct air capture (DAC) or via an optimal mix of point-source capture and DAC when possible (i.e., when concentrated emissions are present); (2) point-source capture does not allow capture of 100% of $CO_2$, hence some amount of DAC is always needed; (3) no carbon-based products (no gray arrows) but only carbon-free products (blue arrows, hydrogen and nitrogen) are present for the production of carbon-free chemicals (c, hydrogen/electrification route); (4) the gray square box receiving the chemical product represents the end-user service; (5) the biomass type is not strictly identified by wood; (6) carbon-free electricity is only reported for the steps with the highest consumption.

capture from concentrated sources to a few hundred for capture from air.[37–40] While considered key in abating the emissions of hard-to-abate industries, CCS routes rely on the continued use of fossil fuels and on the availability of large $CO_2$ storage capacity, which result in social acceptability challenges for CCS deployment.[41]

### *Carbon capture and utilization*

In the carbon capture and utilization (CCU) route, the chemical industry achieves net-zero carbon emissions by substituting the provenience of carbon for C-based chemicals: from the high-energy reduced fossil carbon to the oxidized low-energy carbon in the $CO_2$, which has been previously captured from point-source emitters (via PSC) and/or from the atmosphere (DAC). CCU requires the development of a new chemical industry, organic chemistry, and catalysts that convert $CO_2$ into the targeted C-based product.[42–48] Alternatively, $CO_2$ can be converted into CO-rich synthesis gas (syngas; a mixture of mainly $H_2$, CO, and $CO_2$), $CH_4$, methanol, or dimethyl ether, which is thereafter converted into the targeted carbon products via the BAU route. In all cases, CCU requires low-carbon hydrogen and energy as inputs for product synthesis, as these are not extracted from fossil hydrocarbons any longer. Also, it is worth noting that while permanent $CO_2$ storage is a unique element of CCS, $CO_2$ capture is necessary for both CCS and CCU.

### *Hydrogen/electrification*

The hydrogen route is conceptually similar to the CCU route, but only applies to C-free chemicals such as ammonia. Ammonia production can attain net-zero emissions (in this case it can indeed be decarbonized) by replacing the provenance of the hydrogen atoms: from fossil fuels to water electrolysis using renewable electricity.[21,49,50] Here, the electrification of the chemical industry is the most prominent element,[51,25] no carbon is involved, and no $CO_2$ capture is required. While ammonia can in principle be net zero also by coupling fossil fuels and CCS, the CCS infrastructure would arguably find a better use for hard-to-decarbonize organic chemicals.

### *Biomass utilization*

Biomass contains both the carbon and hydrogen atoms as well as the energy required for the synthesis of chemical products.[52–57] However, the chemical structure of biomass feedstocks is less favorable than that of fossil fuels, for example in terms of higher water content and lower energy content. In the biomass route, $CO_2$ is captured from air via photosynthesis during the biomass growth and then emitted upon synthesis and end-of-life of the biomass-based product, thus resulting in net-zero $CO_2$ emissions.

#### *Integration of carbon recycling*

The carbon recycling route applies mostly to plastics, and considers that a fraction of the chemical products is recycled back to the synthesis plant once it has delivered its service. However, even though recycling rates are maximized, all recycling processes produce residual wastes.[30,26,58] These residual wastes are incinerated, leading to unavoidable $CO_2$ emissions. Therefore, the carbon recycling route must be combined with other net-zero routes to compensate for such emissions and to provide the amount of carbon that cannot be sourced from recycled material. For example, the amount of carbon that does not come from recycled materials can be sourced from fossil fuels, hence requiring coupling of the carbon recycling route with CCS; alternatively, it can be provided in the form of $CO_2$ captured from air via DAC (CCU route) or via biomass (biomass route). Several studies assessed the potential of carbon recycling technologies to mitigate the emissions of plastics production, highlighting the potential to significantly reduce the burden on net-zero production processes[12,19,59–67] and enable plastics production within the planetary boundaries.[9,10]

Finally, it is worth noting that we do not assess routes that are currently under development.[68] These include novel electrochemical synthesis processes for ammonia production,[69–73] plasma-activated approaches,[74] and novel thermochemical processes for drop-in fuels.[75] While these technologies are promising, they will not be able to contribute to the immediate needs of the chemical industry in a world of net-zero $CO_2$ emissions.

## Circularity and demand-side measures

Circularity and demand-side measures are key in the move toward net-zero emissions. In general, reducing the amount of end-products or primary chemicals is crucial to meet net-zero targets, as it leads to a smaller amount of required energy and material feedstock.[9,76,77] Meng et al. present seven planet-compatible routes that combine supply- and demand-side interventions for the entire chemical industry.[9] They show that resource efficiency and circularity measures can reduce the global demand for chemicals by up to 33% and are critical to achieving net-zero emissions while complying with available natural resources.

Circularity and demand-side measures also reduce the impact of chemical products on the environment. For example, an estimated 11 Mt of plastics (about 2% of global production) leak into waterways and oceans every year as a result of ineffective waste management systems,[26,78,79] with estimates for 20 Mt/year in 2050.[29] Thus, plastic recycling is a key measure in preventing negative environmental impacts on the road to net-zero emissions. Meys et al. show that net-zero emission plastics can be achieved by combining biomass and CCU with an effective recycling rate of about 70%.[19] Furthermore, Bachmann et al. show that a climate-optimal plastics industry, which combines current recycling rates with biomass and CCU, transgresses sustainability thresholds by up to four times. Recycling rates higher than 75% would open a safe operating space for sustainable plastics in 2030. Importantly, their analysis shows that sustainable plastics require not only novel technologies but also a fundamental change in our perception of plastics as cheap and disposable products.[10]

Stegmann and colleagues show that a circular bioeconomy that combines plastics recycling with biomass feedstock has the potential to transform plastics into a carbon sink (under a stringent set of technological and socioeconomic conditions) while reducing the reliance of future plastics on biomass feedstock, energy, and land use for landfill.[80] However, it is worth noting that today only about 15% of plastic waste is collected for recycling; of that, 40% is discarded from the recycling process because of its low quality. As a result, actual plastic recycling rates are about 9%.[58,81] With most plastic sent for recycling being downcycled because of its heterogeneous nature, improved recycling technologies and collection processes are needed.[58]

Ammonia demand can be reduced by encouraging plant-based diets, which avoid the conversion from plants to animal products and reduce the nitrogen footprint by reducing food losses and waste and improving nitrogen-use efficiencies.[82] For example, it is estimated that more than 50% of the ammonia-based nitrogen fertilizers are overapplied and not needed to grow crops; they are lost to the environment, contributing to GHG emissions and freshwater eutrophication.[83] Therefore, improved agriculture practices, such as precision agriculture, can reduce ammonia demand and related emissions by half.[84] Nitrogen losses from farm to fork are estimated to be above 40% and are mainly due to harvesting and distribution losses as well as food waste.[27,22] Reducing food waste and improving efficiencies in food supply chains can reduce demand for nitrogen fertilizers, hence ammonia. Finally, transitioning from a linear to a circular economy that captures and recycles nitrogen from waste can moderate the use of resources and the energy required to produce ammonia.[17] Similarly, promoting the use of organic fertilizers such as manure or compost can also reduce ammonia demand.[85] However, organic fertilizers are often more expensive, slower in releasing nutrients, and are not presently capable of supporting the demands of current or future generations.[17,86]

## Key technologies for net-zero chemical production

For all chemical products, all net-zero production routes require multiple technologies and processes (Figure 2). In all cases, some technologies are commercial and already available today, while some are new and need further development.

#### *Novel technologies for chemical synthesis*

Different processes are available for the different routes for the synthesis of all chemicals of interest (see experimental procedures).

*Ammonia*. Conventional production of ammonia ($NH_3$) in BAU and CCS routes is carried out via the Haber-Bosch process. Today, conventional Haber-Bosch processes use natural gas (70%), coal (26%), oil (1%), and electricity (4%) as feedstock.[17]

Various studies have assessed processes to go beyond fossil fuels in ammonia production by using biomass or hydrogen directly.[11,49,50,87–92] Compared with conventional processes, the electrification route relies on the use of renewable energy to produce hydrogen and nitrogen for product synthesis.[50,51,89] In this case, electricity has the potential to provide all the energy requirements, with water replacing methane as the hydrogen source. In contrast, biomass-based ammonia can be produced via gasification processes starting from dry biomass,[87,93] as well as anaerobic digestion starting from wet biomass feedstocks.[92]

*Methanol*. The production of methanol (MeOH) in BAU and CCS routes is carried out via the current industrial process, where CO and $CO_2$ contained in syngas are hydrogenated.[94] Syngas is derived from either natural gas or coal by steam reforming, partial oxidation, or gasification.

In the CCU route, methanol is produced starting from $CO_2$ and hydrogen directly. While direct methanol synthesis is still an open research field, various process simulations have been presented for methanol synthesis from $CO_2$ and hydrogen,[95–103] and the first large plant has recently started operation.[104] In the biomass-based route, methanol production can be carried out via biomass gasification processes.[105]

*High-value chemicals and plastics*. Conventional production of plastics is widely based on oil and natural gas. These are first refined into ethane, propane, and other petrochemical products, which are then transformed into high-value chemicals (ethylene, propylene, benzene, toluene, xylenes) via a cracking process in high-temperature furnaces. The resulting high-value chemicals are combined with a catalyst to produce polymers, which are transformed into plastic products using processes such as extrusion and molding.[29]

The conventional processes for plastics production can be replaced by processes based on the use of $CO_2$, hydrogen, and biomass.[57,19,61,62,80,106] The CCU and biomass routes assume that plastic waste is primarily incinerated; the resulting $CO_2$ emissions are circulated by capturing $CO_2$ from the atmosphere via DAC or biomass, respectively, and by using this $CO_2$ as the feedstock of the plastic production process. Net-zero plastics production can be achieved by combining biomass and CCU with plastics recycling.[19] In this context, various recycling technologies are available and can be combined, including options with high technology readiness level (TRL), such as sorting of plastic packaging waste and subsequent mechanical recycling, and options with low TRL, such as chemical recycling of all plastic waste.[62]

*Low-carbon energy*. This is energy generated with substantially lower GHG emissions than conventional energy based on fossil fuels. Low-carbon electricity can be supplied via renewable energy technologies, such as solar photovoltaic, wind turbines, or hydropower, or via other low-carbon technologies, such as nuclear power and fossil plants with CCS.[76]

Low-carbon heat can be generated via electricity-driven heat pumps or waste heat when low-temperature heat is required, e.g., for solid DAC technologies,[40,107–109] and via C-free fuels (e.g., hydrogen boilers), when high-temperature heat is required, e.g., for liquid DAC technologies[110] or process heat.

All net-zero routes strongly rely on C-free energy, which is a key component of a net-zero chemical industry.[68,111]

*Low-carbon hydrogen*. More than 95% of hydrogen is currently produced via steam methane reforming (SMR) of natural gas, contributing to about 2% of global $CO_2$ emissions.[112] Low-carbon hydrogen can be produced by coupling SMR (or auto-thermal reforming [ATR] and hydrocarbon cracking) with CCS, by using water electrolysis powered by renewable electricity, SMR (or ATR) of biogas produced from anaerobic digestion of biomass, and biomass gasification.[113–115]

*Sustainable biomass*. Despite the lack of a clear and globally accepted definition for sustainable biomass,[116] we define it here as biomass grown without generating additional environmental impacts on the ecosystem (e.g., no loss of biodiversity). Sustainable biomass can consist of waste biomass and residues, such as crop residues, forestry residues, food waste, and livestock manure.[117,118] When no sustainable biomass is available as a feedstock for the production of chemicals, biomass growth requires land, water, and nutrients, which can all compete with agricultural production and ecosystems.[119]

*$CO_2$ capture*. $CO_2$ capture is used to capture the $CO_2$ emissions generated along the entire chemical product chain. $CO_2$ can be captured exclusively from the atmosphere via DAC or via a combination of PSC and DAC when possible. On the one hand, DAC can be geographically decoupled from chemical production plants; hence, it can deal with distributed emissions and can be placed where resources in terms of energy supply and $CO_2$ storage are best available.[120] On the other hand, PSC requires less energy per unit of captured $CO_2$ due to the higher $CO_2$ concentration in the flue gases of the end-of-life processes than in air (i.e., 5%–15% in flue gases vs. 420 ppm in air).[37] When PSC is employed, and given that 100% $CO_2$ removal is hardly feasible, additional DAC capacity would be required to comply with net-zero $CO_2$ emissions. Different combinations of PSC and DAC are possible, based for example on the tradeoff between lower capture costs for PSC and lower transport costs for DAC.

*$CO_2$ storage*. After it is captured, and possibly transported, $CO_2$ can be permanently sequestered in geological formations underground, through carbon capture, transport, and storage supply chains.[121,122] Examples of suitable geological formations are found in North America, e.g., Petra Nova and Boundary Dam,[123,124] in the North Sea, e.g., in Norway, the Netherlands, and the United Kingdom,[125] and in Iceland.[126,127] While $CO_2$ storage in aquifers and in oil and gas reservoirs has been practiced at a commercial scale for decades in the North Sea, North America, Australia, and elsewhere,[128–133] $CO_2$ storage still faces issues concerning the actual availability, accessibility, and acceptance of storage sites.[134,135] Recent assessments indicate that a vast underground storage capacity might be available, i.e., between 7,000 and 55,000 $GtCO_2$, which can be stored worldwide.[136–138]

An alternative to geological storage is given by using and permanently storing $CO_2$ in construction materials, such as concrete, through a carbon capture, utilization, and storage supply chain.[139–143] However, current estimates of storage capacity in C-rich products and building materials are far from the gigaton scale required to achieve a net-zero chemical industry.[141,143]

## COMPARATIVE ASSESSMENT OF NET-ZERO PRODUCTION ROUTES

The comparative assessment of all net-zero routes follows a methodology presented earlier for methanol production,[34] which considers all major steps in the chemical production process, from chemical synthesis to end-of-life, and focuses on energy and $CO_2$ storage requirements, land use, and water consumption (see experimental procedures). Whereas a detailed assessment of net-zero chemicals would require a careful definition of system boundaries and a comprehensive life-cycle assessment (LCA),[144] the simplified framework adopted here provides useful and straightforward insights for the general comparison of the considered net-zero routes (which, for example, do not depend on allocation methods, as in LCA), as highlighted by its application in earlier studies.[34,107,145] Here, we model the available net-zero routes for the production of methanol, ammonia, and plastics by building upon previous assessments for single chemicals and routes.[50,19,89,93,100] A detailed description of the assessment methodology is provided in experimental procedures.

Net-zero routes are assessed and compared in terms of (1) electricity consumption, (2) heat consumption, (3) land use, (4) water consumption, (5) $CO_2$ storage capacity, and (6) residual $CO_2$ emissions in case C-free energy is unavailable. Such indicators are selected because of their relevance in determining the technical and biophysical feasibility of the net-zero routes. All input data required to perform the analysis are provided in a public online repository (see "data and code availability"). Schematics of the processes for all routes and chemicals are shown in Figures 7, 8, and 9 (see experimental procedures).

## Energy consumption

The energy intensity (per ton of produced chemical, Figure 3A) varies greatly across net-zero routes: the CCU/electrification route is characterized by an electricity consumption of about 10 $MWh_e$ per ton of produced methanol and ammonia and about 40 $MWh_e$ per ton of produced plastic. This increase corresponds to a factor of 40–70 compared with BAU production and is mainly associated with the necessity of producing hydrogen. When considering the global production of primary chemicals, this translates into an average electricity consumption of about 17 $PWh_e$ in 2020 and 32 $PWh_e$ in 2050 (Figures 3B and 3C); for comparison, today's yearly global energy consumption for all purposes is 25 $PWh_e$. This raises serious questions about route feasibility and the availability of low-carbon electricity. For example, the use of low-carbon electricity for primary chemicals production might affect the pathway to full decarbonization of other sectors, e.g., the power, transport, or aviation sectors.[145–147] From this perspective, all routes producing C-rich products using DAC may compete with the use of DAC as a negative emissions route[148,149]; similarly, the amount of low-carbon hydrogen required (about 800 $MtH_2$ per year in 2050, from the current global demand of about 90 $MtH_2$) will have to compete with other sectors to supply low-carbon hydrogen.

The other routes result in much smaller electricity consumption, on the same order of magnitude as BAU, except for plastic production from biomass. Here, hydrogen must be produced to complement the amount of hydrogen in the biomass,[19] resulting in an electricity consumption of about 13 $MWh_e$ per ton of plastic.

In all net-zero production routes, the process heat is generated by the main feedstock (namely fossil fuels for BAU and CCS, hydrogen for CCU and electrification, and biomass for the biomass route). The heat consumption reported in Figure 3 is the low-temperature heat (<100°C) required for $CO_2$ capture (see experimental procedures). This is higher for the CCS and CCU routes, where carbon is captured via technology-based solutions (especially when carbon is captured via DAC). When considering the global production of primary chemicals in 2050, this translates into an average heat consumption of about 5 $PWh_t$ and 10 $PWh_t$ for CCS and CCU, respectively, or about 10% and 20% of the current global heat consumption.[76]

## Land and water

Producing net-zero chemicals requires additional amounts of land and water. When achieving net-zero emissions via biomass, the average land use ranges from about 1,600 $m^2$ per ton of ammonia produced to about 3,000 $m^2$ per ton of plastic produced (Figure 3A), which results in an average value of about 4.6 million $km^2$ of land to meet the projected chemical production in 2050 (Figure 3C). This number is significantly higher than BAU (90–150 times) and CCS (40–140 times).

CCU also requires a significant amount of land because of the large electricity consumption, but still 3–7 times smaller than biomass; in fact, CCU is also subject to significant land-use uncertainty, as land use strongly depends on the electricity generation technology, ranging from about 0.5 $m^2/(MWh_e/year)$ for nuclear to about 20 $m^2/(MWh_e/year)$ for solar.[150] Note that here we consider solar, nuclear, and onshore wind as possible electricity sources, while we do not consider offshore wind. Whereas offshore wind would not compete for land against other land uses, the results of the analysis would be similar to the case of nuclear electricity generation (which has limited land use).[150]

Similar considerations apply to water consumption, with biomass consuming from 100 to 10,000 times more water than the other routes and requiring an average of about 5,200 $km^3$ of water for the projected chemicals production in 2050 (Figure 3C). Importantly, biomass growth uses both rainwater (or green water) and surface and/or groundwater (or blue water); the former is used by absorbing the humidity in the soil, whereas the latter is consumed via irrigation.[151] In contrast, CCU, CCS, and BAU routes only use blue water sourced from rivers, lakes, and aquifers. For comparison, today's global water consumption for food production is estimated to be about 7,000 $km^3$ (6,000 $km^3$ green water and 1,000 $km^3$ blue water), whereas all industry sectors combined consume about 100 $km^3$ (blue water only).[119]

## Emissions with current electricity carbon intensity

All considered routes result in net-zero emissions if C-free energy is available, while residual emissions are present when considering current and projected energy carbon intensities (Figure 4A). Considering the low-temperature heat (Figure 3) electrified via heat pumps, the carbon footprint of the chemical industry increases proportionally to the carbon intensity of electricity.

However, different routes are more or less sensitive to the carbon intensity of electricity: The BAU route results in about 3 $tCO_2$ per ton of chemical produced (weighted average of methanol, ammonia. and plastic production), independently of the type of electricity supply, as the largest share of $CO_2$ emissions is due to the use of fossil carbon (Figure 4A). In contrast, the $CO_2$ emissions of the other routes increase significantly with the electricity carbon intensity, with those of the CCU route growing about 17 and 5.5 times faster than those of the CCS and biomass routes, respectively (Figure 4A). This is due to the larger energy consumption of CCU and biomass routes (mostly electricity used for hydrogen production) and is primarily driven by the

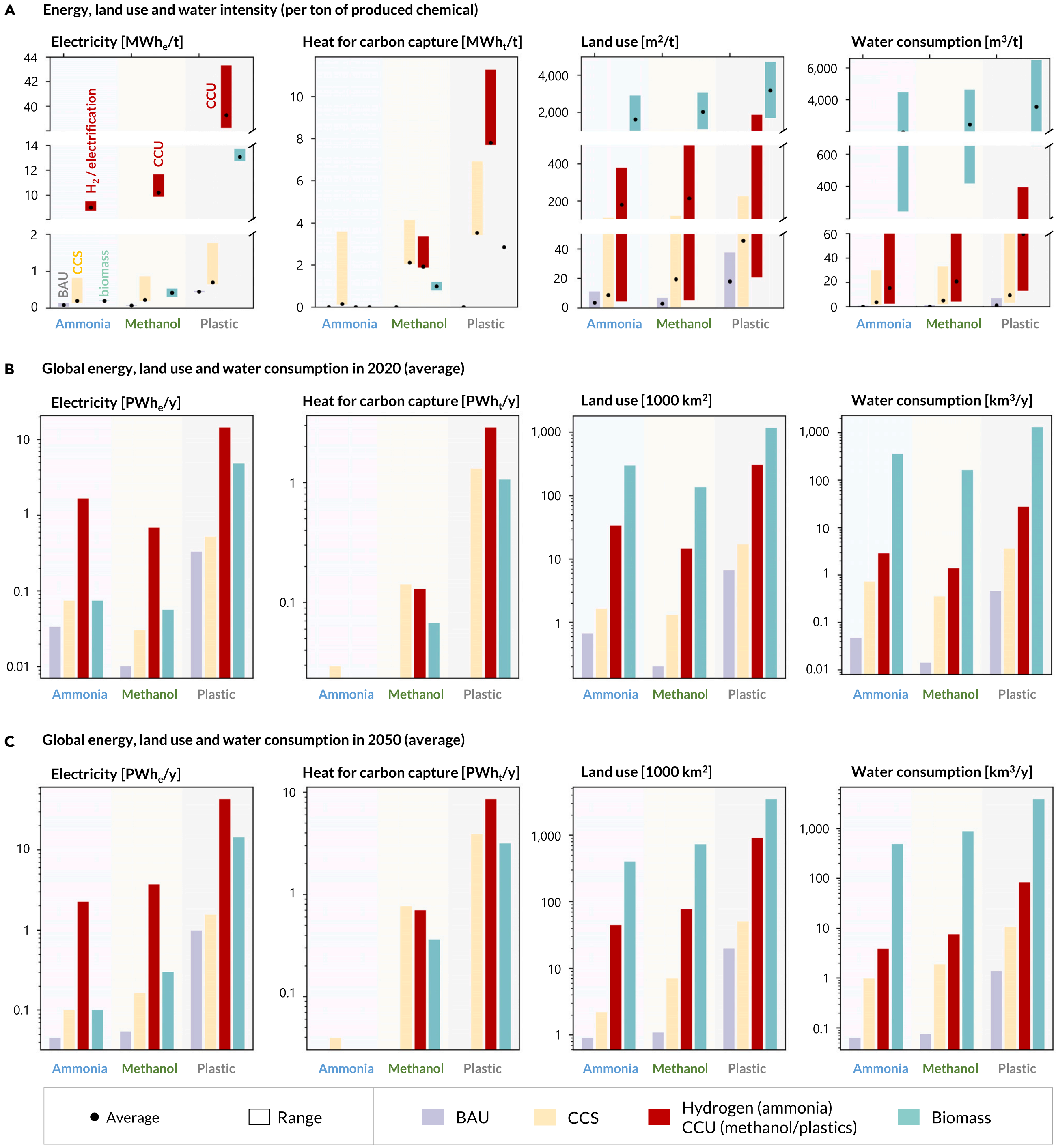

**Figure 3. Comparative assessment of net-zero routes**

Comparative assessment of BAU, CCS, CCU, and biomass routes in terms of (A) electricity, heat, land use, and water consumption intensity (per ton of produced chemical), and (B and C) yearly global electricity, heat, land use, and water consumption in 2020 (B) and 2050 (C); 2050 values are based on projected production of ammonia (250 Mt/year), methanol (360 Mt/year), and plastics (1,100 Mt/year). All routes are considered individually and with no carbon recycling. In (A), average values are represented by black dots, whereas uncertainty ranges are due to different sources of energy (solar, onshore wind, nuclear) and $CO_2$ (combination of point-source and direct air capture) (see experimental procedures). All routes, except BAU, can achieve net-zero emissions as long as carbon-free electricity is available. The reported heat is low-temperature heat required by carbon capture, whereas the process heat is provided by the main feedstock (namely fossil fuels for BAU and CCS, hydrogen for CCU, and biomass for the biomass route).

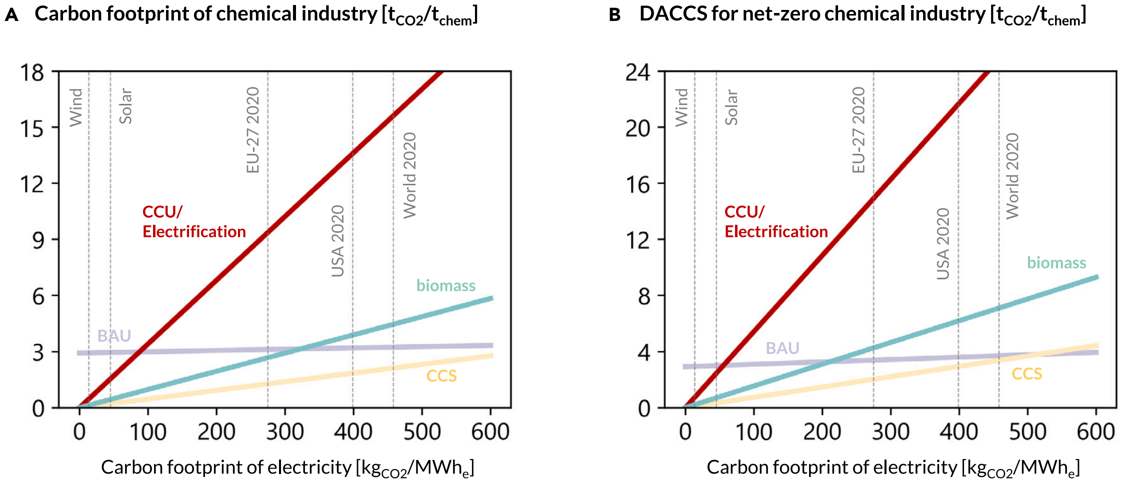

**Figure 4. Residual emissions of the global chemical industry due to non-carbon-free energy**

(A) Specific carbon footprint of the chemical industry and (B) required specific deployment of DAC with $CO_2$ storage (DACCS) to achieve net-zero emissions when adopting BAU, CCS, CCU, and biomass routes as a function of the carbon footprint of electricity. The weighted average carbon footprint of the chemical industry is computed by considering the projected production of chemicals in 2050: ammonia (250 Mt/year), methanol (360 Mt/year), and plastics (1,100 Mt/year). The average carbon intensity is considered for all routes and chemicals. For non-carbon-free electricity, achieving net-zero carbon emissions requires additional carbon dioxide removal, proportionally to the electricity carbon footprint.

production of net-zero plastic, which is more energy-intensive than methanol and ammonia production. This implies that, while today CCU has the potential to reduce the emissions of the chemical industry with respect to BAU in some regions (such as the Scandinavian countries, France, and Switzerland, where the electricity carbon footprint is lower than 100 $gCO_2$/kWh), it would result in higher emissions than BAU in most countries (such as the United States and most European and Asian countries). CCU will reduce the emissions of the chemical industry only if coupled with low-carbon electricity generation (such as dedicated solar and wind installations) and result in lower emissions than BAU when the electricity carbon footprint is smaller than about 90 $gCO_2$/kWh (Figure 4A). Furthermore, even in countries with low-carbon footprints for electricity, CCU will require significant amounts of additional low-carbon electricity generation (Figure 3).

The emissions resulting from a non-C-free energy supply will have to be offset for all routes by deploying negative emissions technologies, such as DAC with $CO_2$ storage (DACCS), resulting in further environmental tradeoffs.[152] Figure 4B shows the amount of DACCS required to achieve net-zero emissions as a function of the carbon footprint of electricity: about 15 $tCO_2$ per ton of chemicals produced via the CCU route must be captured via DAC and permanently sequestered when considering the current average European carbon intensity (2–5 $tCO_2$ per ton of chemicals produced for CCS and biomass routes). DACCS is required also when considering deep electricity decarbonization: 1–7 $tCO_2$ per ton of produced chemicals must still be offset for an electricity carbon intensity of 100 $gCO_2$/kWh; for the current carbon footprint of dedicated solar generation (about 50 $gCO_2$/kWh), the CCU route will still require a similar amount of DACCS as the BAU route. Figure 4B features lines with higher slopes than Figure 4A, because DACCS (like other negative emissions technologies) also requires electricity to operate. Therefore, the impact of the carbon intensity of electricity is greater on the amount of DACCS required (Figure 4B) than on the direct $CO_2$ emissions of the chemical industry (Figure 4A).

From a global perspective, significant improvements are still needed toward low-carbon electricity, with the global average carbon footprint of electricity being about 450 $gCO_2$/kWh[28] and the carbon footprint of solar, wind, hydro, and nuclear electricity ranging between 5 and 100 $gCO_2$/kWh because of their life-cycle impact (wind is on the lower side and solar on the upper side).[150] When complying with net-zero-emissions trajectories, the global carbon footprint of electricity is expected to fall below 100 $gCO_2$/kWh around 2040 and to be approximately 10 $gCO_2$/kWh in 2050.[76]

Finally, the reliance on C-free electricity might be reduced by combining different routes with each other. For example, combining the CCU route with hydrogen production from biomass would reduce the need for C-free electricity, possibly without increasing land use and water consumption if using waste or residue biomass.[153–155]

## IMPACT ON RESOURCES, INFRASTRUCTURES, AND SUPPLY CHAINS

### Competition for natural resources

All net-zero routes might incur tradeoffs in terms of environmental resources, namely land use, water consumption, and availability of sustainable biomass. We assess the consumptions of biomass and water for all net-zero routes, but we compare such consumptions with the biophysical resources of sustainable biomass and freshwater, respectively, because we consider sustainable biomass and freshwater to evaluate the biophysical viability of the net-zero routes. Table 1 reports the global average land use, biomass use, and water consumption required for all routes to achieve a net-zero chemical industry in 2020 and 2050, and puts them into perspective with global resources.

**Table 1. Comparison of available and required natural resources for a net-zero chemical industry**

| | Freshwater ($km^3$/year) | | Land (1,000 $km^2$) | | Biomass (EJ) | |
|---|---|---|---|---|---|---|
| | 2020 | 2050 | 2020 | 2050 | 2020 | 2050 |
| CCS | 4.7 | 13.5 | 19.9 | 59.5 | – | – |
| CCU/$H_2$ | 26.4 | 77.1 | 353 | 1,029 | – | – |
| Biomass | 1,841 | 4,628 | 1,612 | 4,628 | 36 | 101 |
| Anthropogenic activities | 12,400 | | 52,000 | | 50[d] | N/A |
| Biophysical resources[a] | 21,000[b] | | 56,500[c] | | 10[e] | 60[e] |

Land use, sustainable biomass use, and water consumption for all net-zero routes, namely CCS, CCU, and biomass, in 2020 and 2050. Global available resources and resources currently used by anthropogenic activities are reported for comparison. Current anthropogenic activities and available resources are considered also for 2050 (N/A, not available).

[a] Biophysical resources do not consider current anthropogenic activities. Thus, resources availability is computed as the difference between biophysical resources and anthropogenic activities.

[b] Estimate of global availability of blue water[156] and green water.[157]

[c] Highest estimate of unused productive land in 2000.[158]

[d] All biomass used by anthropogenic activities.[159]

[e] Highest estimate of available sustainable biomass, including municipal solid waste.[159,160]

Producing net-zero chemicals significantly increases water consumption compared with BAU, especially for the biomass route (Figure 3 and Table 1). The global freshwater availability per year is about 21,000 $km^3$—about 4,000 $km^3$ of blue water[156] and 17,000 $km^3$ of green water.[157] Of this, current human activities already consume about 12,400 $km^3$ of freshwater per year, with agriculture contributing to about 90%.[157,161] This suggests that a solution purely based on biomass would not be sustainable for the planet, especially when considering the competition with other industrial sectors, which at the moment do not contribute significantly to freshwater consumption, but will need to undergo a transformation similar to that of the chemical industry.[162,163] Similar considerations, but to a lower extent, apply to the CCU route, which also requires a significant amount of freshwater resources mostly due to the water consumption of energy generation (0.1–3 $m^3$/MWh) required to produce hydrogen. Also, the adoption of carbon capture and storage technologies, which are key components of the CCS and CCU routes, could be constrained by water scarcity in various geographical areas.[164]

Similar considerations apply to land use. The biomass and CCU routes require significant land resources, mostly related to the high land-use intensity of biomass (490–1,072 $m^2$/tbio) and energy production (0.5–40 $m^2$/[MWh/year]). In 2050, the biomass and CCU net-zero routes will need about 100% and 20% of the total available land worldwide.[158] Biomass and energy generation might compete with each other and with fertile arable land needed to grow food for the growing and more affluent global population. However, the integration of large-scale wind turbines on agricultural land has become common practice, with little effect on crop production.[165] The same is true for solar panels when adopted in the form of agrivoltaics installation, which can increase resource-use efficiency, agricultural productivity, low-carbon electricity generation, and reduced water use.[166] Overall, global land scarcity should be mitigated by using resources that do not create additional impacts on land and water resources, such as waste biomass or residues[117,153] and offshore wind. However, sustainable biomass resources are also limited, and our results show that a solution only based on biomass would not be feasible even when limiting the primary chemical production to the current level (Table 1).

While current estimates suggest that no inherent physical or geographical limitations are present from the perspective of materials and minerals depletion,[9] similar considerations might apply when considering the large requirements of renewable energy generation and hydrogen production.[76,167] In fact, the transition from a fossil-based energy system to one based on renewable energy results in a significant need for materials and minerals, especially when considering the competition across sectors.[168,169] This might translate into a shift of the geopolitical equilibria, where supply chains stop being dominated by fossil fuels and start being dominated by minerals, with solar supply chains playing a major role.[170]

## Land and water scarcity at country level

While global figures provide a good picture of the challenges ahead, the availability of land and water resources varies significantly with the geographical location.[171,172] This calls for local analyses to assess the technical and environmental viability of a net-zero chemical industry. While a site-specific analysis would ideally be performed, no data are available on the exact location of chemical plants globally; this suggests the need for better data to refine the analysis of land and water scarcity on a local scale. Figure 5 shows the current land and water scarcity worldwide, on a country basis, as well as the additional land and water scarcity incurred when achieving a net-zero chemical industry via the considered production route (see experimental procedures). The additional land and water scarcity induced by the chemical industry refer to the country-specific production of chemicals in 2020. This represents an optimistic scenario from the perspective of chemical demand growth (i.e., no growth), although it does not consider possible demand reductions due to circularity schemes or demand-side measures. The same analysis for the projected chemical production in 2050 is shown in Figure 10 (see experimental procedures).

A scarcity factor greater than 1 implies that more water or land is used than is supported by the environment in a sustainable way. For example, land scarcity is observed when anthropogenic activities entail deforestation (note that this can be observed in countries with large surface areas), and water scarcity can be observed when more water is used than is regenerated by hydrological basins after accounting for environmental flows (as is already the case in the MENA region, India, and China). Figure 5 also reports the values of land and water scarcity for selected countries. For example, the United States does not face current land and water scarcity (both factors are lower than 1), while land scarcity is observed in Brazil (1.05) and water scarcity is observed in China (1.04).

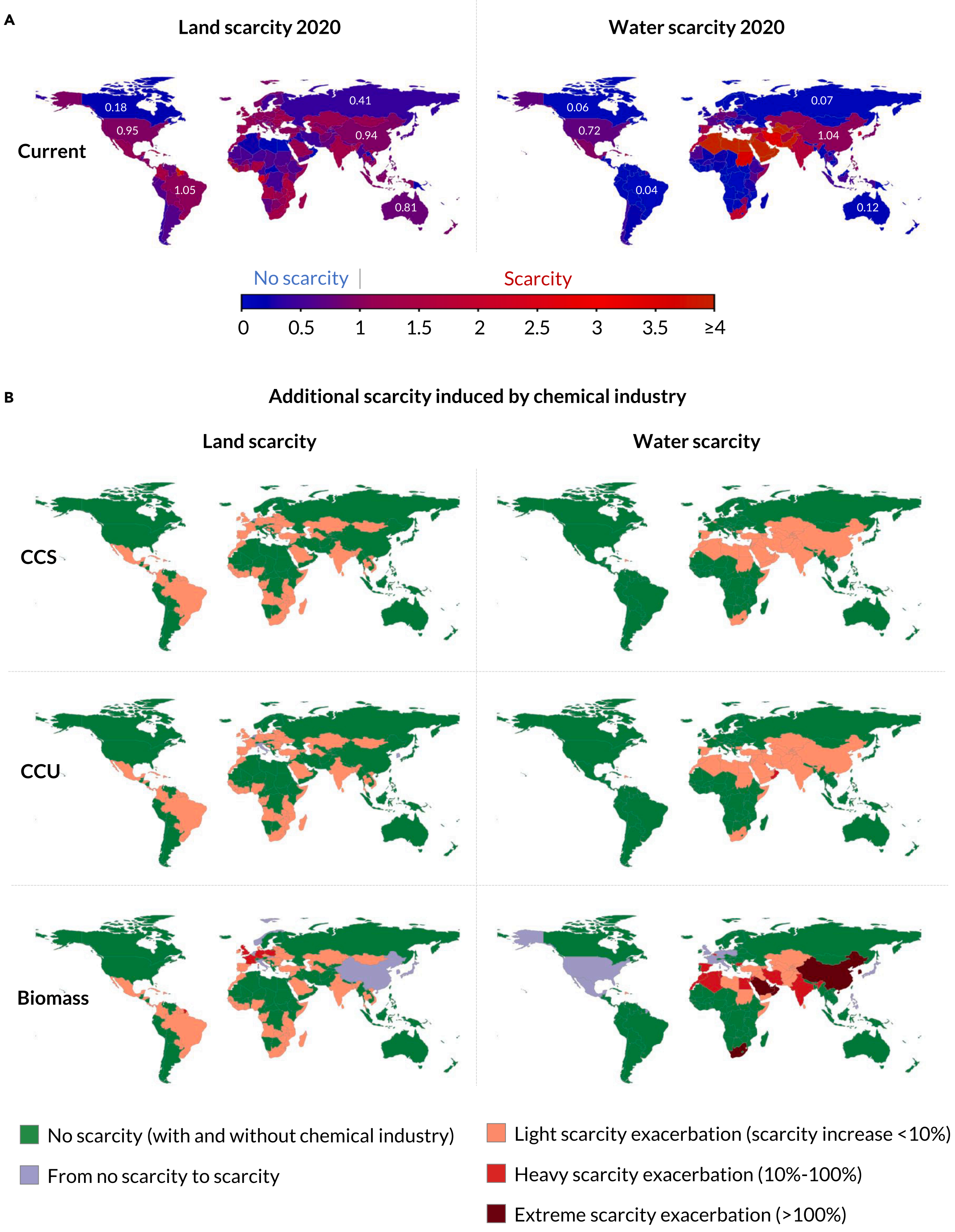

**Figure 5. Country-level water and land scarcity for net-zero chemical industry**

Current scarcity (A) and additional scarcity induced by net-zero chemical industry (B). Land and water scarcity are defined by the land-use-to-availability ratio and the water-consumption-to-availability ratio, respectively (see experimental procedures). Values of land and water scarcity are reported for selected countries. Land use and water consumption of the chemical industry are computed on the basis of the country-specific chemical production in 2020 (optimistic scenario, zero growth of today's chemical industry). See Figure 10 (and experimental procedures) for land and water scarcity under 2050 production. Values of current scarcity are reported for selected countries.

When considering the chemical production in 2020, land scarcity in Europe would be slightly exacerbated (i.e., countries that already experience scarcity would see an increase in scarcity smaller than 10%) by the CCS and CCU routes, whereas it would be heavily exacerbated (i.e., increase in scarcity up to 100%) by the biomass route (Figure 5). Furthermore, the biomass route would cause most European countries to experience water scarcity, which is not the case today. The CCS and CCU routes would slightly exacerbate land scarcity in other countries too, such as Brazil, Mexico, India, Central Asia countries, and southern African countries; they would also slightly exacerbate water scarcity in the MENA region, Central Asia countries, India, and China; water scarcity would be significantly exacerbated in Oman due to its significant ammonia and plastic production. The biomass route would lead to land scarcity in China and would heavily or extremely exacerbate water scarcity in the MENA region, India, China, and South Africa. This shows that China, India, and the vast majority of Europe will not be able to achieve a net-zero chemical industry with local resources via the biomass route, being limited by both land and water (Figure 5). Overall, Europe and Japan are much more limited by land resources than water resources. In contrast, MENA countries and India are much more limited by water resources than land resources. In fact, none of the net-zero routes can be pursued in these regions because of pronounced water scarcity. This might reshape the international trade of ammonia and hydrogen, with the production of chemicals moving from countries with significant fossil resources (BAU) to countries with abundant land and water resources.

## Synergies among production and demand-side measures

The analysis presented above highlights a critical competition for land and water resources when considering individual net-zero production routes. This underlines two key aspects: the necessity of integrating multiple routes and the necessity of combining net-zero production processes with circularity measures, such as plastics recycling, and with demand-side measures aimed at improving end-use efficiency and reducing the production volume of chemical products.

While we do not tackle the optimal combination of multiple net-zero routes, which depends on various objectives (e.g., costs, energy, land, and water consumption) and is most likely affected by a variety of socio-political parameters, we investigate the impact of plastics recycling on land and water resources. Figure 6 shows the reduction in land and water scarcity that can be achieved by combining the CCS, CCU, and biomass routes with plastics recycling. We consider a recycling rate of 75%[10]; while this is much higher than the current global average recycling rate (about 9%[58]), we choose it to show the potential of maximizing recycling rates for reducing the environmental impacts of global plastics production. Also, we focus on plastics recycling, as plastics production is the greatest contributor to the emissions and environmental impact of the chemical industry.

The effect of recycling is visible in the biggest plastics producer, namely China, where carbon recycling eliminates land scarcity induced by the chemical industry and reduces water scarcity; the United States, where carbon recycling allows us to eliminate the water scarcity induced by the chemical industry; and Europe, where carbon recycling eliminates (e.g., Italy, France, the Netherlands, and United Kingdom) or reduces (e.g., Germany, Poland, and Spain) the land and water scarcity induced by the chemical industry (Figure 6). Countries with predominant methanol and ammonia production might reduce the land and water scarcity induced by the chemical industry by adopting corresponding demand-side measures (see "circularity and demand-side measures").

## Carbon and hydrogen infrastructures and supply chains

A net-zero world where CCS and CCU routes are deployed on a large scale requires the deployment of $CO_2$ and hydrogen infrastructures and supply chains to connect sources and sinks of $CO_2$ and hydrogen. More specifically, achieving net-zero emissions via CCS will require a significant storage capacity: about 5 $GtCO_2$ in 2050, or 200 $km^3$ of storage volume, when considering CCS as an individual route. This storage capacity is much smaller (three orders of magnitude) than estimated available storage resources, with lower estimates on the order of 7,000 $GtCO_2$.[136,138] However, current storage facilities store about 40 $MtCO_2$ per year globally,[132] calling for a much wider deployment of CCS installations to comply with the quantities required to achieve net-zero emissions. This holds true for today's values of demand for chemicals.

In the CCS route, $CO_2$ is collected from large-scale point sources or absorbed from the atmosphere at multiple locations. Wei et al. suggested a global layout for CCS in line with a 2°C climate target, where 80% of all $CO_2$ sources worldwide can be connected to a storage site within 300 km.[173] However, longer source-to-sink distances will likely be needed by CCS early movers, owing to the currently limited options for permanently storing $CO_2$ underground.[121,122,174–176] For example, the $CO_2$ captured by countries in Central Europe will need to travel more than 1,000 km to the currently available storage hubs.[125,127] Moreover, whereas pipelines are the preferable option to transport volumes of $CO_2$ larger than 1 $MtCO_2$ per year,[121] and hence will likely be needed for the large-scale $CO_2$ network required by a net-zero chemical industry, CCS pioneers are currently demonstrating smaller supply chains (on the order of 1 $ktCO_2$ per year) by adopting different transport technologies, such as isotainers carried via trains, trucks, barges, and ships.[127,176]

Similarly, achieving net-zero emissions via CCU requires designing, developing, and deploying hydrogen infrastructures and supply chains alongside $CO_2$ ones.[112,115] Various analyses have been carried out to design hydrogen supply chains and to optimally connect sources and sinks of hydrogen,[177–179] with the latter being represented here by CCU chemical industries. For both hydrogen and $CO_2$ supply chains, tradeoffs exist between centralized and distributed hydrogen production and $CO_2$ capture.[179–181] The former benefits from lower costs due to larger scales in the case of hydrogen production, and from greater capture efficiencies due to higher concentrations in the case of $CO_2$ capture; the latter benefits from lower transport costs, since the sources of hydrogen and $CO_2$ can be placed directly at the sink locations.

Both the $CO_2$ and hydrogen infrastructures, which essentially do not exist today, could be shared by multiple routes toward a net-zero chemical industry, and potentially by multiple

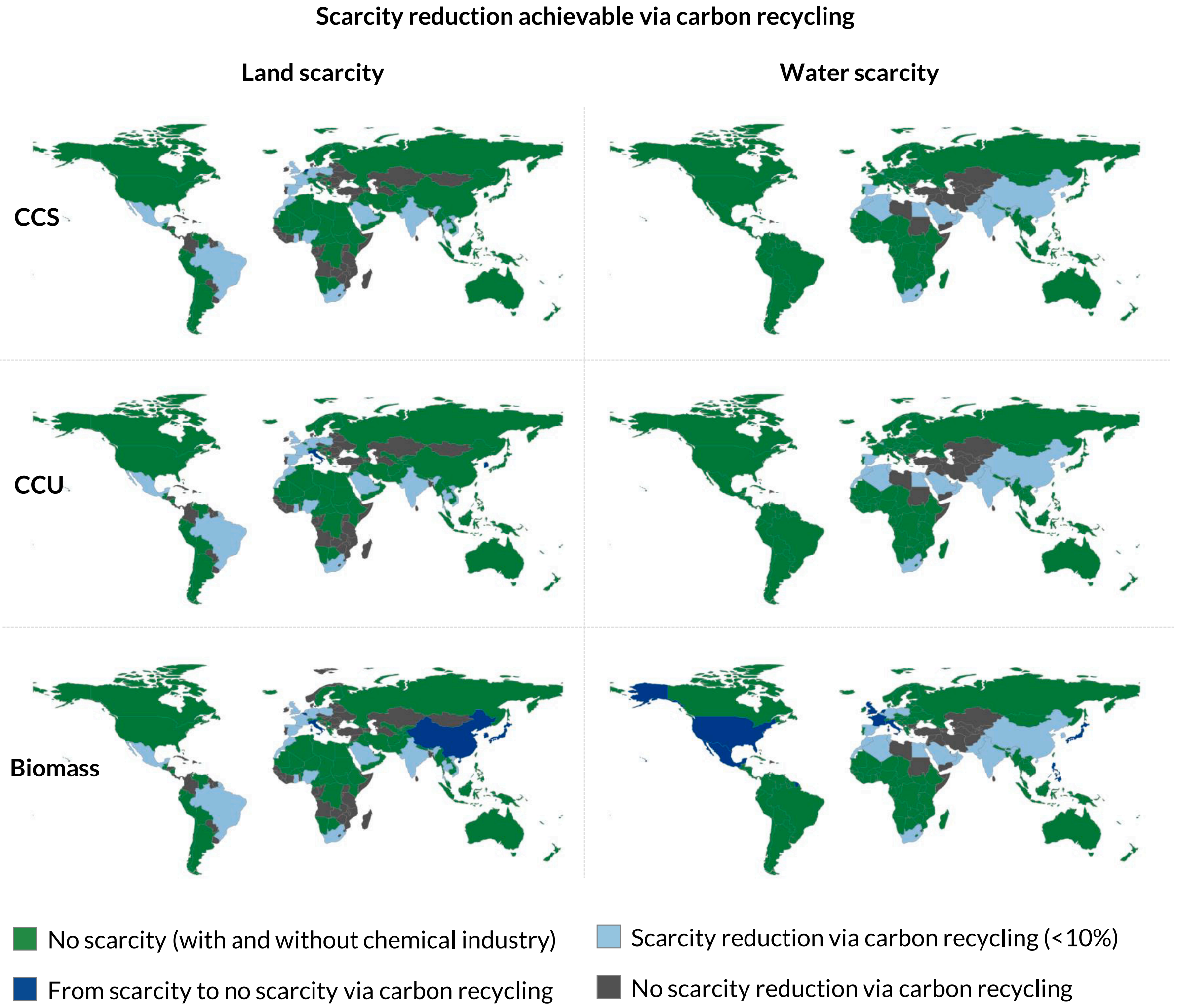

**Figure 6. Country-level reduction of land and water scarcity achievable via plastics recycling**

A maximal recycle rate of 75% is considered for all countries and is combined with the CCS, CCU, and biomass routes. The effects of plastics recycling are most visible in the most relevant plastics producers, such as China, the United States, and Europe. Land use and water consumption of the chemical industry are computed on the basis of the country-specific chemical production in 2020 (i.e., an optimistic scenario, with zero growth of today's chemical industry).

sectors and countries. Thus, they will need to be designed while accounting for the optimal rollout, full-scale deployment, and real-world constraints imposed by all relevant stakeholders. To this end, two challenges co-exist: (1) the optimal configuration of the relevant infrastructures when at full-scale; and (2) the most efficient way to develop such infrastructures during the transition period.

## Industry transition and policy landscape

The global chemical industry generates US$4.7 trillion in revenues annually, representing about 4% of global GDP, and directly employs over 15 million people.[182] Overall, the chemical industry strongly relies on capital-intensive and long-lived assets and requires significant investments to change its business models and operations.[76,183] Any structural changes to be in place by 2050 require action soon, preferably now.[183]

Some encouraging signals arrive from industry players. For example, Lange provides an industry perspective on the transformation of petrochemicals, where he addresses challenges related to shifting hydrocarbon stock, climate change, and circular economy, and highlights the importance of all net-zero routes.[30] The analysis proposes a possible evolution of the transition driven by the costs of available technologies. More specifically, Lange suggests that in the first phase of the transition, the chemical industry is expected to have access to abundant fossil hydrocarbons as the energy sectors phase out of fossil fuels; in this phase, the $CO_2$ emissions can be abated through CCS to avoid paying rising $CO_2$ prices. Then, as fossil fuels are phased out from all sectors, low-carbon feedstocks will be adopted, first through biochemical processes and, eventually, through CCU. However, CCU will need to develop significantly to be able to compete with biomass. All these routes will need to be coupled by increasing recycling rates.[30]

While several leading chemical companies started to set credible climate mitigation targets,[184] creating acceptance and demand for low-carbon industrial products will need multiple diverse actions, including education, changes to industry standards, procurement policies, financial incentives, and low-carbon product standards.[5,185,186] Furthermore, achieving net-zero emissions will not be entirely under the direct control of the chemical industry. For instance, the impact and effectiveness of circularity and demand-side measures depend on the combination of other societal and technological changes—at the moment only 9% of plastic is recycled,[58] and only about 20% of fertilizers produced from ammonia actually end up in crops that feed the global population.[187–189] Moreover, the extensive modification and building of plants will require equipment manufacturers, engineering, procurement, and construction industries to expand their capacity significantly.

From the perspective of the policy landscape, work to abate the emissions of the chemical industry is being undertaken with an increased sense of urgency worldwide,[190] with commonalities being observed across the globe[183]: (1) low-carbon hydrogen generation (especially via water electrolysis) receives the most attention and policy support among key technologies to enable a net-zero chemical industry; (2) electrification is also receiving significant attention, with low-carbon electricity generation being a top priority for most countries; (3) biomass utilization currently receives the least policy support together with waste processing and circularity, although both are likely to receive additional policy support in the future, moving away from fossil feedstock.[191,192]

## REMAINING GAPS AND OUTLOOK

This study assesses the potential and challenges of available technology routes to transform the chemical industry in a world of net-zero $CO_2$ emissions. More specifically, we assess the technical and environmental feasibility of net-zero routes at a country level, hence resolving geographical differences in assessing and designing a net-zero chemical industry. However, further research is needed to perform site-specific assessments, i.e., with a resolution higher than the country level, as biophysical resources can be unevenly distributed within countries. High-resolution assessment will allow us to better quantify the environmental and biophysical impacts of net-zero chemicals on local natural resources and ecosystems as well as the potential for efficiency gains through process integration. This calls for a data-acquisition campaign on the exact locations and characteristics of chemical plants globally, which is currently unavailable.

Furthermore, we stress the importance of combining net-zero routes with each other and with circularity and demand-side measures, and we find that the potential of integrated solutions will differ regionally based on local resources. Further research is needed to determine optimal combinations of net-zero routes that minimize the resource scarcity induced by a net-zero chemical industry. Furthermore, while we focus only on the evolution of the chemical industry, future research efforts will be devoted to investigating the co-evolution of the chemical and energy sectors.

While our study suggests a potential reshaping of international trading of chemicals, further research will be needed to determine global layouts of chemical supply chains that minimize the costs, the environmental and biophysical impacts of a transition to net-zero emissions, and maximization of the security of supply. However, such a reshaping will likely be driven not only by available resources but also by chemical demand, economic interests, and existing technological know-how.

Finally, building a chemical industry compatible with a net-zero world requires structural changes within and beyond the chemical industry itself and immediate action. Indeed, some of the technologies required for the transition to net-zero emissions still have low TRL (e.g., related to CCU-based chemical synthesis and chemical plastics recycling). However, much technology is already available and could be deployed globally—for example, recycling technologies. While such technologies might feature costs higher than BAU, we can and should take action now while still working on the open issues.

Overall, while some work to abate the emissions of the chemical industry is being currently undertaken, the efforts to support key technologies toward net-zero emissions, such as carbon capture, low-carbon hydrogen, carbon storage, biomass utilization, plastics recycling, and efficiency improvements in the use of nitrogen fertilizers, must be drastically and quickly scaled up through global coordination.

## EXPERIMENTAL PROCEDURES

### Resource availability

#### *Lead contact*

Further information and requests should be directed to the lead contact, Paolo Gabrielli (gapaolo@ethz.ch).

#### *Materials availability*

This study did not generate new unique materials.

#### *Data and code availability*

All data needed to reproduce the results have been deposited at Mendeley Data and are available at the following DOI: https://doi.org/10.17632/9ghcvh2dmb.1

### Modeling approach

The analyses presented in "comparative assessment of net-zero production routes" and "impact on resources, infrastructures, and supply chains" build upon the framework introduced earlier for net-zero methanol production.[34] This is a simplified assessment framework, which does not perform a thorough LCA but considers all major steps in the chemical production process from product synthesis to end-of-life; this implies neglecting the energy consumption and $CO_2$ emissions associated with the manufacturing process of the technologies of interest. All the net-zero routes of interest are considered, namely BAU, CCS, CCU (for methanol and plastics), electrification (for ammonia), and biomass. The assessment procedure for all chemicals is described below. A schematic of the processes enabling the net-zero production of ammonia, methanol, and plastics is shown for all routes in Figures 7, 8, and 9, respectively, which also report the energy and mass balances. The numerical results for all routes and chemicals, together with all input data required to perform the analysis and reproduce the results, are provided in a public online repository (see "data and code availability").

### Net-zero production routes

#### *Ammonia ($NH_3$)*

Conventional production of ammonia ($NH_3$) in BAU and CCS routes is carried out via the Haber-Bosch process. Today, conventional Haber-Bosch processes use natural gas (70%), coal (26%), oil (1%), and electricity (4%) as feedstock,[17] with the methane-fed process resulting in the highest energy efficiency and the lowest carbon emissions.[17] This is a highly integrated process, but can be broken down into two main functional steps: hydrogen production from methane and ammonia synthesis by the Haber-Bosch reaction.

Here, we assume a production process based on natural gas, which uses about 0.49 tons of fossil carbon (tC), or 0.65 tons of natural gas, to produce 1 ton of ammonia ($tNH_3$).[17] By applying stoichiometry, this results in $CO_2$ emissions of about 1.8 $tCO_2/tNH_3$ for the BAU ammonia production process. In this

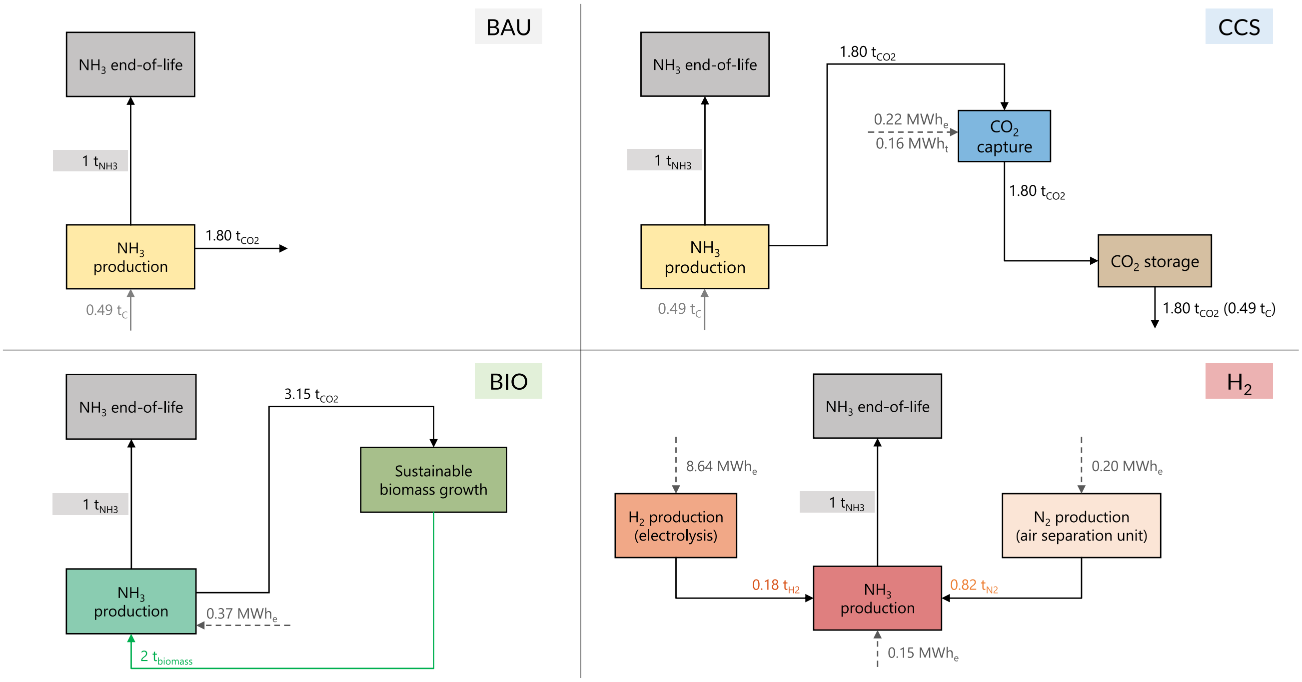

**Figure 7. Process modeling for ammonia production**
Schematic representation of the BAU, CCS, hydrogen ($H_2$), and biomass routes for the production of ammonia. All routes, except BAU, can achieve net-zero emissions if carbon-free electricity is available. Material and energy balances refer to the production of 1 ton of ammonia (1 $t_{NH3}$).

process, $CO_2$ must be removed through the Benfield or Selexol processes (which consists of primary and secondary SMR and two-stage water-gas shift) to enable the synthesis of ammonia in the Haber-Bosch reaction. This $CO_2$ is possibly utilized (e.g., for urea production) but is eventually vented to the atmosphere. A similar fate is undergone by the diluted $CO_2$ present in the exhaust gases resulting from the use of fossil fuels for energy inputs.

In contrast, when adopting CCS, both the concentrated $CO_2$ resulting from the use of the fossil feedstock and the diluted $CO_2$ in the exhaust gases

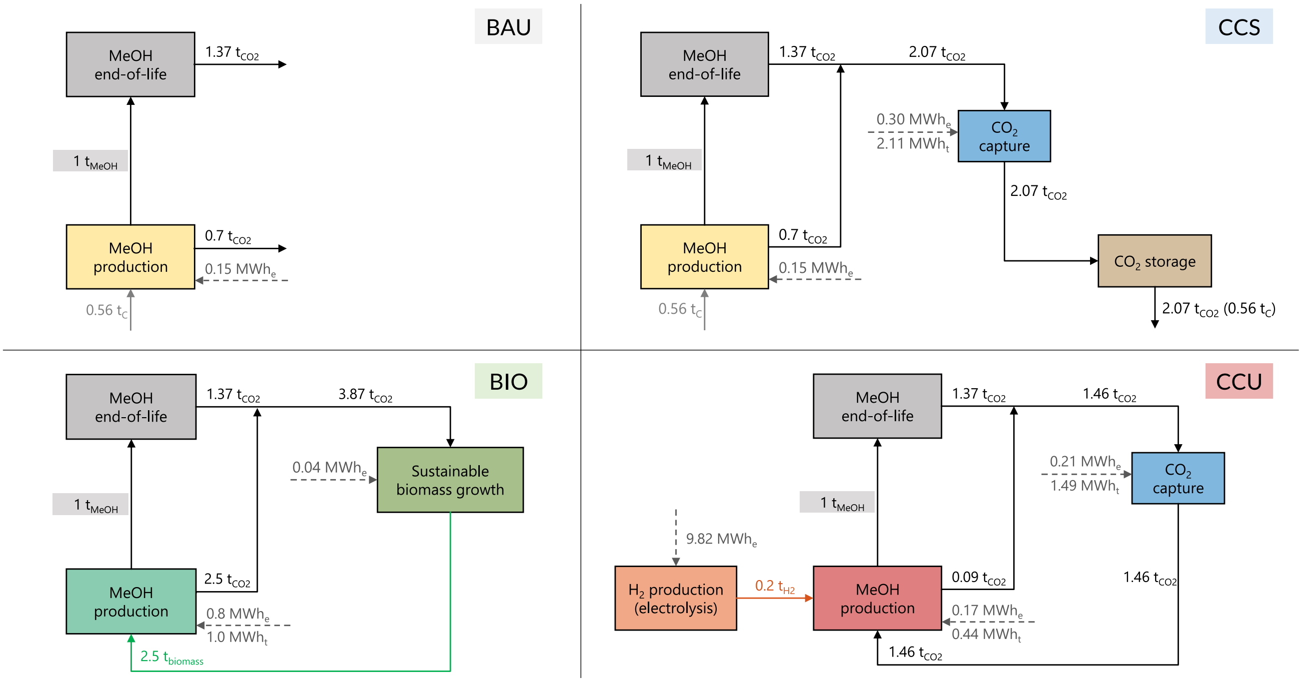

**Figure 8. Process modeling for methanol production**
Schematic representation of the BAU, CCS, CCU, and biomass routes for the production of methanol. All routes, except BAU, can achieve net-zero carbon emissions if carbon-free electricity is available. Material and energy balances refer to the production of 1 ton of methanol (1 $t_{MeOH}$).

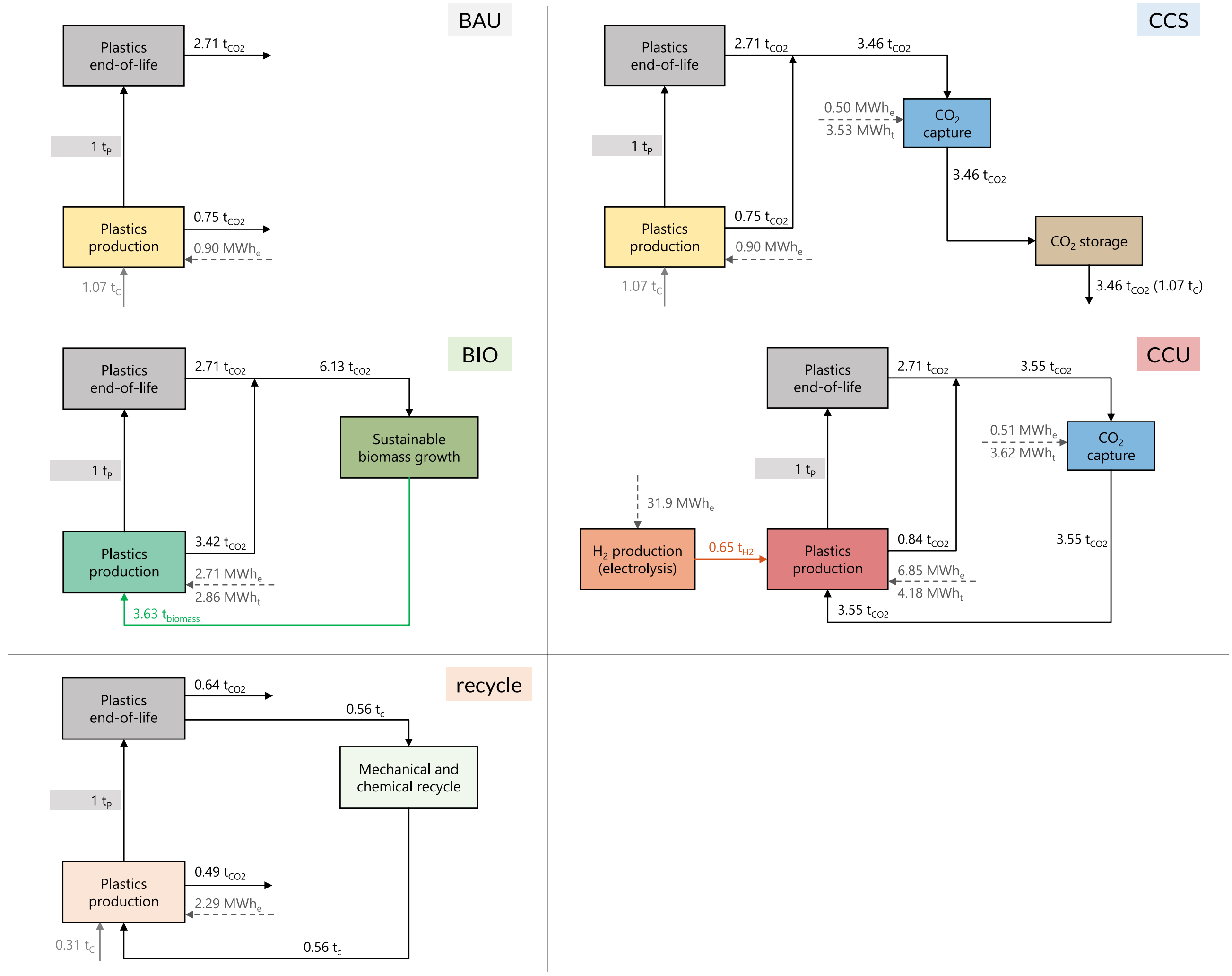

**Figure 9. Process modeling for plastics production**

Schematic representation of the BAU, CCS, CCU, and biomass routes for the production of plastics. All routes, except BAU and recycle, can achieve net-zero carbon emissions if carbon-free electricity is available. Material and energy balances refer to the production of 1 ton of plastics (1 $t_P$). The recycle route can help toward net-zero emissions by reducing the demand for plastics.

resulting from fossil fuel combustion are captured, transported to a permanent storage site, and permanently sequestered. Here we assume $CO_2$ transport via pipeline, which results in negligible $CO_2$ emissions, and we neglect $CO_2$ emissions associated with $CO_2$ transport and storage.[121]

For the BAU route, we consider an average electricity consumption of 0.18 MWh/$tNH_3$ (ranging from 0.08 MWh/$tNH_3$ for SMR to 0.28 MWh/$tNH_3$ for ATR). Such electricity consumption is added to the energy inputs provided by fossil fuels and is needed to run auxiliary components.[17]

When implementing CCS (coupling the Selexol process for concentrated $CO_2$ and amine absorption for diluted $CO_2$ in the exhaust gases), the overall $CO_2$ capture process has a capture efficiency of about 95%, with 5% of the emissions still escaping to the environment and being captured back with DAC to achieve net-zero $CO_2$ emissions.[17] Here, we consider an electricity consumption of 0.1 $MWh_e/tCO_2$ for compressing the $CO_2$ to transport- and storage-ready conditions (110 bar), and a heat consumption of 0.94 $MWh_t/tCO_2$ for the amine absorption process; no additional heat is required by the Selexol process, thanks to heat integration. It is worth noting that, for all routes, no $CO_2$ is emitted during ammonia end-of-life processes.

Both the electrification and the biomass routes are still based on the Haber-Bosch process, which is either fully electrified or fueled by biomass. The electrification route relies on the use of renewable energy to produce hydrogen, 0.18 $tH_2$, and nitrogen, 0.82 $tN_2$, for product synthesis. Hydrogen is produced via water electrolysis with an average efficiency of 70% (range 65%–75%), hence an electricity consumption of 47.6 $MWh_e/tH_2$ (range 44.4–51 $MWh_e/tH_2$)[17,193] and 0.24 $MWh_e/tN_2$.[89] No carbon, hence no direct $CO_2$ emissions, is present in this case. Biomass-based ammonia production is carried out via a gasification process starting from dry wood chips, with 43% carbon content and a lower heating value of about 17 MJ/kg. The process uses an average of 2 tons of biomass (range 1.3–2.7 tbio/$tNH_3$) and 0.37 $MWh_e$ to produce 1 ton of ammonia.[87,93] By applying stoichiometry, the process results in direct $CO_2$ emissions of 3.15 $tCO_2/tNH_3$. This $CO_2$ is removed by biomass while growing; the value of biomass uptake is computed to close the carbon balance and is equal to 1.58 $tCO_2$/tbio. An average land-use factor of 800 $m^2$/[tbio/year] (range 490–1,072 $m^2$/[tbio/year]) and an average electricity consumption of 0.01 $MWh_e$/tbio (range 0.005–0.015 $MWh_e$/tbio) are considered for the managed biomass growth installation.

### *Methanol (MeOH)*

Production of methanol in BAU and CCS routes is carried out via the current industrial process, where CO and $CO_2$ contained in a synthesis gas (or syngas, a mixture of mainly $H_2$, CO, and $CO_2$) are hydrogenated in the presence of a Cu-ZnO-$Al_2O_3$ catalyst at 5–10 MPa and 200°C–300°C.[94] Syngas can be derived from either natural gas or coal by steam reforming, partial oxidation, or gasification (with the latter being used especially in the case of heavy oils or solid carbonaceous materials). Here we assume a production process based on natural gas, which uses an average of 0.56 tons of fossil carbon to produce 1 ton of methanol, resulting in $CO_2$ emissions of 0.70 $tCO_2$/tMeOH.[34,100,194]

After methanol has delivered its service, it is disposed of and carbon returns to the atmosphere. By applying stoichiometry, methanol end-of-life results in $CO_2$ emissions of 1.37 $tCO_2$/tMeOH. In the BAU route, the overall $CO_2$ emissions resulting from methanol synthesis and end-of-life are vented to the atmosphere. In contrast, when applying CCS, $CO_2$ emissions are captured, transported to a permanent storage site, and permanently sequestered. Here we consider the possibility of capturing all $CO_2$ emissions via a point-source process, but we consider an overall capture efficiency ranging from 0%, where all the $CO_2$ is emitted in a distributed fashion and captured back from the atmosphere via DAC, to 90%, where 90% of the $CO_2$ emissions is captured from point-source emitters and the rest via DAC.

For the BAU route, we consider an average electricity consumption of 0.15 MWh/tMeOH to run auxiliary components.[100] The same electricity and heat requirements described above are used for CCS.

For the CCU route, the process presented by Pérez-Fortes and co-workers (in line with the other studies) is taken here as a reference. It uses 1.46 $tCO_2$, 0.2 $tH_2$, 0.17 $MWh_e$, and 0.44 $MWh_t$ to produce 1 ton of methanol.[100] Similar to the CCS route, the required $CO_2$ is captured from a combination of point-source emitters (with the overall capture efficiency ranging from 0% to 90%) and DAC. CCU-based methanol synthesis results in $CO_2$ emissions of 0.09 $tCO_2$/tMeOH (resulting in overall emissions of 1.46 $tCO_2$/tMeOH when considering methanol end-of-life, respecting stoichiometry).

Finally, biomass-based methanol production can be carried out via gasification processes starting from wood chips with an average carbon content of 43% and a lower heating value of 17 MJ/kg.[34,105] It uses 2.5 tons of dry biomass, 0.8 $MWh_e$, and 1 $MWh_t$ to produce 1 ton of MeOH.[105,195] By applying stoichiometry, we derive the direct $CO_2$ emissions of the synthesis process, 2.5 $tCO_2$/tMeOH, and the value of biomass uptake, 1.55 $tCO_2$/tbio.

### *Plastics*

The production of plastics covers C-based chemicals, plastics, and plastic wastes, with silicone and other non-carbon plastics being excluded. All intermediate products needed during the production of plastics (including ammonia and methanol) are included. The chemicals and plastics covered in the analysis are described in the supporting information of a study from Meys et al.[19] Following up on that work, average values across all produced plastics are used here. Plastics include: polyamide 6, polyamide 66, polyethylene terephthalate (PET) pellets (fiber-grade), PET pellets (bottle-grade), polyacrylonitrile fiber, high-density polyethylene, low-density polyethylene, linear low-density polyethylene, polypropylene, general-purpose polystyrene, polystyrene, flexible polyurethane, rigid polyurethane, and polyvinyl chloride. Chemicals and plastics production and end-of-life are based on detailed LCA technology models, which consider full energy and mass balances.

Multiple plastics recycling technologies are considered: sorting of plastic packaging waste and subsequent mechanical recycling, and chemical recycling of all plastic waste.[19] A maximal recycle rate of 75% is considered.

## Assessment of $CO_2$ emissions

For all chemicals, the carbon intensity of all routes considers the contribution of the production processes described above; C-free electricity is considered for the analysis presented in "energy consumption" and "land and water," whereas a variable carbon footprint of electricity is discussed in "emissions with current electricity carbon intensity." For all chemicals *i*, and for all routes *j*, the total $CO_2$ emissions, $C_{i,j}$, are computed as (Equation 1)

$$C_{i,j} = P_i(\varepsilon_{i,j} + \zeta_{i,j} + \alpha_{i,j}\gamma), \qquad \text{(Equation 1)}$$

where $P_i$ is the amount of chemical *i* produced (1 ton when computing intensity values, see Figures 3A, 7, 8, and 9); $\varepsilon_{i,j}$ and $\zeta_{i,j}$ quantify the direct $CO_2$ emissions of production and end-of-life processes, respectively, for chemical *i* and route *j*; $\alpha_{i,j}$ is the specific electricity consumption of production route *j* for chemical *i*; $\gamma$ is the carbon intensity of electricity generation (which depends on the considered generation technology and is treated here as a parameter, see Figure 4). Note that here we considered solar, nuclear, and onshore wind as possible electricity sources, while we do not consider offshore wind. The considered electricity sources cover a wide range of life-cycle $CO_2$ emissions, land use, and water consumption.[150]

The net $CO_2$ emissions resulting from chemical production are non-zero only for the BAU route. For all net-zero routes, the residual $CO_2$ emissions are offset via DAC (which also requires energy to operate). The amount of required DAC to achieve net-zero emissions, $D_{i,j}$, is computed as (Equation 2)

$$D_{i,j} = (C_{i,j} + C_{i,j}\gamma\lambda)\gamma, \qquad \text{(Equation 2)}$$

where $\lambda$ is the amount of electricity required to capture 1 ton of $CO_2$ via DAC. This is the sum of the electricity consumption and electrified heat consumption of DAC. For the calculations, we consider a DAC technology based on solid sorbents (e.g., Climeworks' technology). We consider an electricity consumption of 0.35 $MWh/tCO_2$ (which already includes 0.1 $MWh/tCO_2$ for $CO_2$ compression for making it ready for transport and storage) and a heat consumption of 1.75 $MWh/tCO_2$.[40] Heat is required at low temperatures (around 100°C) and can be supplied via heat pumps (coefficient of performance of 4[196]), resulting in $\lambda = 0.79$ $MWh/tCO_2$.

For all routes and chemicals, the total energy consumption is given by the sum of the contributions of chemical production and DAC.

## Geospatial analysis of land and water scarcity

The land use and water consumption induced by the chemical industry are computed for all routes and all chemicals on a country level. They are obtained by considering country-specific production of chemicals, and the impact of electricity production (solar, onshore wind, nuclear), hydrogen production, DAC, and biomass; the total electricity production, the amounts of required hydrogen, DAC, and biomass are multiplied by the corresponding land and water intensity factors.

It is worth noting that we decided to use chemical production instead of chemical demand. This is because our analysis focuses on the production of net-zero chemicals, and mostly refers to the production of chemicals in 2020. Considering chemicals consumption instead, might make sense in the case of a future reshaping of the chemical industry. However, such a reshaping would be driven not only by chemical demand but also by economic interests, existing technology know-how, and other considerations going beyond the scope of the current analysis.

Country-specific production of chemicals is obtained by using different databases from the International Fertilizer Association[197] and Statista.[198]

Country-specific land and water scarcity are defined as the ratio of land use and water consumption to usable land and water resources, respectively.[199] Land data are taken from the Food and Agriculture Organization of the United Nations (FAO) for the year 2020.[200] This is the most up-to-date information on land availability and use for all countries worldwide. Available land is computed by subtracting forest land from the land area of a country. Usable land is assumed to be 70% of the available land; this fraction ensures that the global value of usable land is in line with previous estimates.[158] First, current land scarcity, $\varphi_k$, is computed by only considering current agricultural activities. For all countries *k*, this is computed as (Equation 3)

$$\varphi_k = \frac{M_k}{0.7(A_k - F_k)}, \qquad \text{(Equation 3)}$$

where $M_k$, $A_k$, and $F_k$ are the agricultural land, the land area, and the forest land of country *k*, respectively. The additional land scarcity induced by the chemical industry is computed by considering the land required to produce chemical *i* via route *j* in country *k*, $L_{i,j,k}$. The resulting overall land scarcity, $\omega_{i,j,k}$, is calculated as (Equation 4)

$$\omega_{i,j,k} = \frac{M_k + L_{i,j,k}}{0.7(A_k - F_k)}. \qquad \text{(Equation 4)}$$

Similarly, water data are taken from FAO data for 2020.[201] Usable water resources are obtained by subtracting environmental flow requirements from the total available renewable water resources. Environmental flow requirements are considered to be 80% of the total renewable water resources, according to the presumptive environmental flow standard; the remaining 20% can be considered as water available for human use without affecting the integrity of downstream water-dependent ecosystems.[199,202] First, current water scarcity, $\psi_k$, is calculated by considering the total human-induced freshwater withdrawal, which accounts for current anthropogenic activities (such as agriculture, energy, industry, and domestic sectors). For all countries *k*, this is computed as (Equation 5)

$$\psi_k = \frac{H_k}{0.2T_k}, \qquad \text{(Equation 5)}$$

where $T_k$ indicates the total renewable water resources and $H_k$ total human-induced freshwater withdrawal. The additional water scarcity induced by the chemical industry is computed by considering the water required to produce

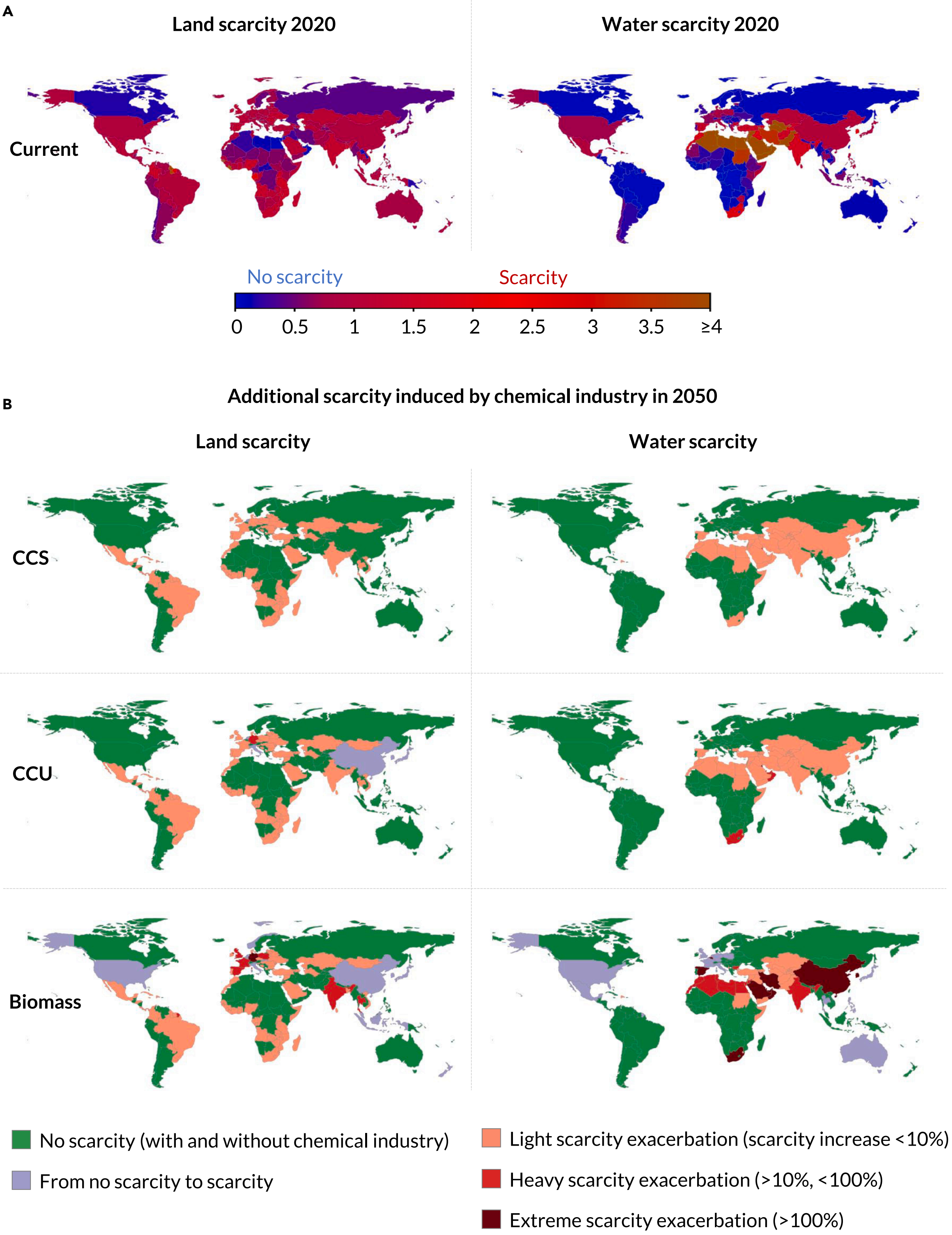

**Figure 10. Country-level water and land scarcity for net-zero chemical industry in 2050**

Current scarcity (A) and scarcity induced by net-zero chemical industry (B). Land and water scarcity are defined by the land-use-to-availability ratio and the water-consumption-to-availability ratio, respectively. Land use and water consumption are computed on the basis of country-specific production of chemicals in 2050; this is obtained by scaling the country-specific production in 2020 by the average global projected values for 2050.

chemical *i* via route *j* in country *k*, $W_{i,j,k}$. The resulting overall water scarcity, $\mu_{i,j,k}$, is calculated as (Equation 6)

$$\mu_{i,j,k} = \frac{H_k + W_{i,j,k}}{0.2T_k} \quad . \text{(Equation 6)}$$

Figure 10 shows the current land and water scarcity worldwide on a country basis, as well as the additional land and water scarcity incurred when achieving a net-zero chemical industry via the considered production routes. The additional land and water scarcity induced by the chemical industry refer to the country-specific production of chemicals in 2050 (values for 2020 are shown in Figure 5).

## ACKNOWLEDGMENTS

The research published in this report was partially carried out with the support of the Swiss Federal Office of Energy as part of the SWEET PATHFNDR project. The research of P.G. was partially funded by the Swiss National Science Foundation exchange grant no. 214037, for his research stay at the Department of Global Ecology at Carnegie Institution for Science. The authors bear sole responsibility for the conclusions and the results.

## AUTHOR CONTRIBUTIONS

Conceptualization, formal analysis, data curation, visualization, writing – original draft, P.G.; Methodology: P.G. with input from L.R.; Writing – review and editing: all authors; Funding acquisition, P.G.

## DECLARATION OF INTERESTS

The authors declare no competing interests.

## REFERENCES

1. Rogelj, J., Popp, A., Calvin, K.V., Luderer, G., Emmerling, J., Gernaat, D., Fujimori, S., Strefler, J., Hasegawa, T., Marangoni, G., et al. (2018). Scenarios towards limiting global mean temperature increase below 1.5 °C. Nat. Clim. Change *8*, 325–332. https://doi.org/10.1038/s41558-018-0091-3.
2. Guardian, T. (2022). The 1977 White House Climate Memo that Should Have Changed the World.
3. IPCC (2021). Summary for policymakers. In Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change, V. Masson-Delmotte, P. Zhai, A. Pirani, S.L. Connors, C. Péan, S. Berger, N. Caud, Y. Chen, L. Goldfarb, and M.I. Gomis, et al., eds. (Cambridge University Press), pp. 3–32. https://doi.org/10.1017/9781009157896.001.
4. Davis, S.J., Lewis, N.S., Shaner, M., Aggarwal, S., Arent, D., Azevedo, I.L., Benson, S.M., Bradley, T., Brouwer, J., Chiang, Y.-M., et al. (2018). Net-zero emissions energy systems. Science *360*, eaas9793. https://doi.org/10.1126/science.aas9793.
5. Woodall, C.M., Fan, Z., Lou, Y., Bhardwaj, A., Khatri, A., Agrawal, M., McCormick, C.F., and Friedmann, S.J. (2022). Technology options and policy design to facilitate decarbonization of chemical manufacturing. Joule *6*, 2474–2499. https://doi.org/10.1016/j.joule.2022.10.006.
6. Financial Time. (2022). Chemicals: Core to a Net Zero Future.
7. Brudermüller, M. (2020). How to Build a More Climate-Friendly Chemical Industry.
8. World Economic Forum (2021). Towards Net-Zero Emissions: Policy Priorities for Deployment of Low-Carbon Emitting Technologies in the Chemical Industry.
9. Meng, F., Wagner, A., Kremer, A.B., Kanazawa, D., Leung, J.J., Goult, P., Guan, M., Herrmann, S., Speelman, E., Sauter, P., et al. (2023). Planet-compatible pathways for transitioning the chemical industry. Proc. Natl. Acad. Sci. USA *120*. e2218294120. https://doi.org/10.1073/pnas.2218294120.
10. Bachmann, M., Zibunas, C., Hartmann, J., Tulus, V., Suh, S., Guillén-Gosálbez, G., and Bardow, A. (2023). Towards circular plastics within planetary boundaries. Nat. Sustain. https://doi.org/10.1038/s41893-022-01054-9.
11. D'Angelo, S.C., Cobo, S., Tulus, V., Nabera, A., Martín, A.J., Pérez-Ramírez, J., and Guillén-Gosálbez, G. (2021). Planetary boundaries analysis of low-carbon ammonia production routes. ACS Sustain. Chem. Eng. *9*, 9740–9749. https://doi.org/10.1021/acssuschemeng.1c01915.
12. Galán-Martín, Á., Tulus, V., Díaz, I., Pozo, C., Pérez-Ramírez, J., and Guillén-Gosálbez, G. (2021). Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries. One Earth *4*, 565–583. https://doi.org/10.1016/j.oneear.2021.04.001.
13. Ioannou, I., Galán-Martín, Á., Pérez-Ramírez, J., and Guillén-Gosálbez, G. (2022). Trade-offs between sustainable development goals in carbon capture and utilisation. Energy Environ. Sci. https://doi.org/10.1039/D2EE01153K.
14. CEFIC (2021). Finland. https://cefic.org/a-pillar-of-the-european-economy/landscape-of-the-european-chemical-industry/finland/.
15. IEA (2021). Chemicals.
16. Cabernard, L., Pfister, S., Oberschelp, C., and Hellweg, S. (2021). Growing environmental footprint of plastics driven by coal combustion. Nat. Sustain. *5*, 139–148. https://doi.org/10.1038/s41893-021-00807-2.
17. IEA (2021). Ammonia Technology Roadmap.
18. IRENA (2021). Innovation Outlook (Renewable Methanol).
19. Meys, R., Kätelhön, A., Bachmann, M., Winter, B., Zibunas, C., Suh, S., and Bardow, A. (2021). Achieving net-zero greenhouse gas emission plastics by a circular carbon economy. Science *374*, 71–76. https://doi.org/10.1126/science.abg9853.
20. 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. https://doi.org/10.1021/acs.est.7b04573.
21. Rosa, L., and Gabrielli, P. (2023). Energy and food security implications of transitioning synthetic nitrogen fertilizers to net-zero emissions. Environ. Res. Lett. *18*, 014008. https://doi.org/10.1088/1748-9326/aca815.
22. Smil, V. (2002). Nitrogen and food production: proteins for human diets. Ambio *31*, 126–131. https://doi.org/10.1579/0044-7447-31.2.126.
23. Erisman, J.W., Sutton, M.A., Galloway, J., Klimont, Z., and Winiwarter, W. (2008). How a century of ammonia synthesis changed the world. Nat. Geosci. *1*, 636–639. https://doi.org/10.1038/ngeo325.
24. Bodirsky, B.L., Popp, A., Lotze-Campen, H., Dietrich, J.P., Rolinski, S., Weindl, I., Schmitz, C., Müller, C., Bonsch, M., Humpenöder, F., et al. (2014). Reactive nitrogen requirements to feed the world in 2050 and potential to mitigate nitrogen pollution. Nat. Commun. *5*, 3858. https://doi.org/10.1038/ncomms4858.
25. Zhao, F., Fan, Y., Zhang, S., Eichhammer, W., Haendel, M., and Yu, S. (2022). Exploring pathways to deep de-carbonization and the associated environmental impact in China's ammonia industry. Environ. Res. Lett. *17*, 045029. https://doi.org/10.1088/1748-9326/ac614a.
26. Geyer, R., Jambeck, J.R., and Law, K.L. (2017). Production, use, and fate of all plastics ever made. Sci. Adv. *3*, e1700782. https://doi.org/10.1126/sciadv.1700782.
27. Ritchie, H., and Roser, M. (2020). $CO_2$ and Greenhouse Gas Emissions.
28. IEA (2021). World Energy Model.
29. IEA (2018). The Future of Petrochemicals.
30. Lange, J.-P. (2021). Towards circular carbo-chemicals – the metamorphosis of petrochemicals. Energy Environ. Sci. *14*, 4358–4376. https://doi.org/10.1039/D1EE00532D.
31. Höhne, N., Gidden, M.J., den Elzen, M., Hans, F., Fyson, C., Geiges, A., Jeffery, M.L., Gonzales-Zuñiga, S., Mooldijk, S., Hare, W., and Rogelj, J. (2021). Wave of net zero emission targets opens window to meeting the Paris Agreement. Nat. Clim. Change *11*, 820–822. https://doi.org/10.1038/s41558-021-01142-2.
32. Net Zero Tracker (2022). Net Zero Stocktake 2022: Assessing the Status and Trends of Net Zero Target Setting across Countries, Sub-national Governments and Companies (New Clim. Institute, Oxford Net zero, energy clim. Intell. Unit data-driven EnviroLab). https://www.zerotracker.net/analysis/net-zero-stocktake-2022/.
33. Schlögl, R., Abanades, C., Aresta, M., Azapagic, A., Blekkan, E.A., Cantat, T., Centi, G., Duic, N., El Khamlichi, A., Hutchings, G., and Mazzotti, M. (2018). Novel Carbon Capture and Utilisation technologies: research and climate aspects. https://doi.org/10.26356/CARBONCAPTURE.
34. 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. https://doi.org/10.1021/acs.iecr.9b06579.
35. IPCC (2022). In Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change P, R. Shukla, J. Skea, R. Slade, A. Al Khourdajie, R. van Diemen, D. McCollum, M. Pathak, S.

Some, P. Vyas, and R. Fradera, et al., eds.. https://doi.org/10.1017/9781009157926.

36. Jones, N. (2022). Net-zero Goals in Chemical Industry Could Shift Energy Demand. Factset. https://insight.factset.com/net-zero-goals-in-chemical-industry-could-shift-energy-demand.

37. Bui, M., Adjiman, C.S., Bardow, A., Anthony, E.J., Boston, A., Brown, S., Fennell, P.S., Fuss, S., Galindo, A., Hackett, L.A., et al. (2018). Carbon capture and storage (CCS): the way forward. Energy Environ. Sci. *11*, 1062–1176. https://doi.org/10.1039/C7EE02342A.

38. Kearns, D., Liu, H., and Consoli, C. (2021). Technology Readiness and Costs of CCS.

39. Wang, X., and Song, C. (2020). Carbon capture from flue gas and the atmosphere: a perspective. Front. Energy Res. *8*. https://doi.org/10.3389/fenrg.2020.560849.

40. IEA (2022). Direct Air Capture.

41. Paltsev, S., Morris, J., Kheshgi, H., and Herzog, H. (2021). Hard-to-Abate Sectors: the role of industrial carbon capture and storage (CCS) in emission mitigation. Appl. Energy *300*, 117322. https://doi.org/10.1016/j.apenergy.2021.117322.

42. Beller, M., Centi, G., and Sun, L. (2017). Chemistry future: priorities and opportunities from the sustainability perspective. ChemSusChem *10*, 6–13. https://doi.org/10.1002/cssc.201601739.

43. Aresta, M., and Nocito, F. (2019). Large scale utilization of carbon dioxide: from its reaction with energy rich chemicals to (Co)-processing with water to afford energy rich products. Opportunities and barriers. In An Economy Based on Carbon Dioxide and Water (Springer International Publishing), pp. 1–33. https://doi.org/10.1007/978-3-030-15868-2_1.

44. Aresta, M. (2019). Carbon dioxide utilization: the way to the circular economy. Greenhouse Gas. Sci. Technol. *9*, 610–612. https://doi.org/10.1002/ghg.1908.

45. Centi, G., Iaquaniello, G., and Perathoner, S. (2019). Chemical engineering role in the use of renewable energy and alternative carbon sources in chemical production. BMC Chem. Eng. *1*, 5. https://doi.org/10.1186/s42480-019-0006-8.

46. Centi, G., and Perathoner, S. (2020). Chemistry and energy beyond fossil fuels. A perspective view on the role of syngas from waste sources. Catal. Today *342*, 4–12. https://doi.org/10.1016/j.cattod.2019.04.003.

47. Huo, J., Wang, Z., Oberschelp, C., Guillén-Gosálbez, G., and Hellweg, S. (2023). Net-zero transition of the global chemical industry with $CO_2$-feedstock by 2050: feasible yet challenging. Green Chem. *25*, 415–430. https://doi.org/10.1039/D2GC03047K.

48. Zimmerman, J.B., Anastas, P.T., Erythropel, H.C., and Leitner, W. (2020). Designing for a green chemistry future. Science *367*, 397–400. https://doi.org/10.1126/science.aay3060.

49. Wang, L., Xia, M., Wang, H., Huang, K., Qian, C., Maravelias, C.T., and Ozin, G.A. (2018). Greening ammonia toward the solar ammonia refinery. Joule *2*, 1055–1074. https://doi.org/10.1016/j.joule.2018.04.017.

50. Smith, C., Hill, A.K., and Torrente-Murciano, L. (2020). Current and future role of Haber–Bosch ammonia in a carbon-free energy landscape. Energy Environ. Sci. *13*, 331–344. https://doi.org/10.1039/C9EE02873K.

51. Schiffer, Z.J., and Manthiram, K. (2017). Electrification and decarbonization of the chemical industry. Joule *1*, 10–14. https://doi.org/10.1016/j.joule.2017.07.008.

52. Holmgren, K.M., Berntsson, T., Andersson, E., and Rydberg, T. (2012). System aspects of biomass gasification with methanol synthesis – process concepts and energy analysis. Energy *45*, 817–828. https://doi.org/10.1016/j.energy.2012.07.009.

53. Holmgren, K.M., Andersson, E., Berntsson, T., and Rydberg, T. (2014). Gasification-based methanol production from biomass in industrial clusters: characterisation of energy balances and greenhouse gas emissions. Energy *69*, 622–637. https://doi.org/10.1016/j.energy.2014.03.058.

54. Cespi, D., Passarini, F., Vassura, I., and Cavani, F. (2016). Butadiene from biomass, a life cycle perspective to address sustainability in the chemical industry. Green Chem. *18*, 1625–1638. https://doi.org/10.1039/C5GC02148K.

55. Niziolek, A.M., Onel, O., Guzman, Y.A., and Floudas, C.A. (2016). Biomass-based production of benzene, toluene, and xylenes via methanol: process synthesis and deterministic global optimization. Energy Fuels *30*, 4970–4998. https://doi.org/10.1021/acs.energyfuels.6b00619.

56. Carvalho, L., Furusjö, E., Kirtania, K., Wetterlund, E., Lundgren, J., Anheden, M., and Wolf, J. (2017). Techno-economic assessment of catalytic gasification of biomass powders for methanol production. Bioresour. Technol. *237*, 167–177. https://doi.org/10.1016/j.biortech.2017.02.019.

57. Winter, B., Meys, R., Sternberg, A., and Bardow, A. (2022). Sugar-to-What? An environmental merit order curve for biobased chemicals and plastics. ACS Sustain. Chem. Eng. *10*, 15648–15659. https://doi.org/10.1021/acssuschemeng.2c03275.

58. Syberg, K. (2022). Beware the false hope of recycling. Nature *611*, S6. https://doi.org/10.1038/d41586-022-03645-0.

59. Hermann, B.G., Blok, K., and Patel, M.K. (2007). Producing bio-based bulk chemicals using industrial biotechnology saves energy and combats climate change. Environ. Sci. Technol. *41*, 7915–7921. https://doi.org/10.1021/es062559q.

60. Posen, I.D., Jaramillo, P., Landis, A.E., and Griffin, W.M. (2017). Greenhouse gas mitigation for U.S. plastics production: energy first, feedstocks later. Environ. Res. Lett. *12*, 034024. https://doi.org/10.1088/1748-9326/aa60a7.

61. 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. https://doi.org/10.1073/pnas.1821029116.

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

63. Altman, R. (2021). The myth of historical bio-based plastics. Science *373*, 47–49. https://doi.org/10.1126/science.abj1003.

64. Kakadellis, S., and Rosetto, G. (2021). Achieving a circular bioeconomy for plastics. Science *373*, 49–50. https://doi.org/10.1126/science.abj3476.

65. Korley, L.T.J., Epps, T.H., Helms, B.A., and Ryan, A.J. (2021). Toward polymer upcycling—adding value and tackling circularity. Science *373*, 66–69. https://doi.org/10.1126/science.abg4503.

66. Meys, R., Frick, F., Westhues, S., Sternberg, A., Klankermayer, J., and Bardow, A. (2020). Towards a circular economy for plastic packaging wastes – the environmental potential of chemical recycling. Resour. Conserv. Recycl. *162*, 105010. https://doi.org/10.1016/j.resconrec.2020.105010.

67. Schwarz, A.E., Ligthart, T.N., Godoi Bizarro, D., De Wild, P., Vreugdenhil, B., and van Harmelen, T. (2021). Plastic recycling in a circular economy; determining environmental performance through an LCA matrix model approach. Waste Manag. *121*, 331–342. https://doi.org/10.1016/j.wasman.2020.12.020.

68. Mallapragada, D.S., Dvorkin, Y., Modestino, M.A., Esposito, D.V., Smith, W.A., Hodge, B.-M., Harold, M.P., Donnelly, V.M., Nuz, A., Bloomquist, C., et al. (2023). Decarbonization of the chemical industry through electrification: barriers and opportunities. Joule *7*, 23–41. https://doi.org/10.1016/j.joule.2022.12.008.

69. Soloveichik, G. (2019). Electrochemical synthesis of ammonia as a potential alternative to the Haber–Bosch process. Nat. Catal. *2*, 377–380. https://doi.org/10.1038/s41929-019-0280-0.

70. Kyriakou, V., Garagounis, I., Vourros, A., Vasileiou, E., and Stoukides, M. (2020). An electrochemical haber-bosch process. Joule *4*, 142–158. https://doi.org/10.1016/j.joule.2019.10.006.

71. Wu, Z.-Y., Karamad, M., Yong, X., Huang, Q., Cullen, D.A., Zhu, P., Xia, C., Xiao, Q., Shakouri, M., Chen, F.-Y., et al. (2021). Electrochemical ammonia synthesis via nitrate reduction on Fe single atom catalyst. Nat. Commun. *12*, 2870. https://doi.org/10.1038/s41467-021-23115-x.

72. Chen, Z., Ma, X., Yu, W., Wu, L., and Xie, Z. (2021). Measuring the similarity of building patterns using Graph Fourier transform. Earth Sci. Inform. *14*, 1953–1971. https://doi.org/10.1007/s12145-021-00659-6.

73. Du, H.-L., Chatti, M., Hodgetts, R.Y., Cherepanov, P.V., Nguyen, C.K., Matuszek, K., MacFarlane, D.R., and Simonov, A.N. (2022). Electroreduction of nitrogen at almost 100% current-to-ammonia efficiency. Nature *609*, 722–727. https://doi.org/10.1038/s41586-022-05108-y.

74. Winter, L.R., and Chen, J.G. (2021). N2 fixation by plasma-activated processes. Joule *5*, 300–315. https://doi.org/10.1016/j.joule.2020.11.009.

75. Schäppi, R., Rutz, D., Dähler, F., Muroyama, A., Haueter, P., Lilliestam, J., Patt, A., Furler, P., and Steinfeld, A. (2022). Drop-in fuels from sunlight and air. Nature *601*, 63–68. https://doi.org/10.1038/s41586-021-04174-y.

76. IEA (2021). Net Zero by 2050.

77. Saygin, D., and Gielen, D. (2021). Zero-emission pathway for the global chemical and petrochemical sector. Energies *14*, 3772. https://doi.org/10.3390/en14133772.

78. Jambeck, J.R., Geyer, R., Wilcox, C., Siegler, T.R., Perryman, M., Andrady, A., Narayan, R., and Law, K.L. (2015). Plastic waste inputs from land into the ocean. Science *347*, 768–771. https://doi.org/10.1126/science.1260352.

79. Lau, W.W.Y., Shiran, Y., Bailey, R.M., Cook, E., Stuchtey, M.R., Koskella, J., Velis, C.A., Godfrey, L., Boucher, J., Murphy, M.B., et al. (2020).

Evaluating scenarios toward zero plastic pollution. Science *369*, 1455–1461. https://doi.org/10.1126/science.aba9475.

80. Stegmann, P., Daioglou, V., Londo, M., van Vuuren, D.P., and Junginger, M. (2022). Plastic futures and their $CO_2$ emissions. Nature *612*, 272–276. https://doi.org/10.1038/s41586-022-05422-5.

81. Rana, K. (2022). This Is How to Ensure Sustainable Alternatives to Plastic.

82. Houlton, B.Z., Almaraz, M., Aneja, V., Austin, A.T., Bai, E., Cassman, K.G., Compton, J.E., Davidson, E.A., Erisman, J.W., Galloway, J.N., et al. (2019). A world of cobenefits: solving the global nitrogen challenge. Earth's Future *7*, 1–8. https://doi.org/10.1029/2019EF001222.

83. Zhang, X., Zou, T., Lassaletta, L., Mueller, N.D., Tubiello, F.N., Lisk, M.D., Lu, C., Conant, R.T., Dorich, C.D., Gerber, J., et al. (2021). Quantification of global and national nitrogen budgets for crop production. Nat. Food *2*, 529–540. https://doi.org/10.1038/s43016-021-00318-5.

84. Sharma, L., and Bali, S. (2017). A review of methods to improve nitrogen use efficiency in agriculture. Sustainability *10*, 51. https://doi.org/10.3390/su10010051.

85. MacLaren, C., Mead, A., van Balen, D., Claessens, L., Etana, A., de Haan, J., Haagsma, W., Jäck, O., Keller, T., Labuschagne, J., et al. (2022). Long-term evidence for ecological intensification as a pathway to sustainable agriculture. Nat. Sustain. *5*, 770–779. https://doi.org/10.1038/s41893-022-00911-x.

86. Barbieri, P., Pellerin, S., Seufert, V., Smith, L., Ramankutty, N., and Nesme, T. (2021). Global option space for organic agriculture is delimited by nitrogen availability. Nat. Food *2*, 363–372. https://doi.org/10.1038/s43016-021-00276-y.

87. Gilbert, P., Alexander, S., Thornley, P., and Brammer, J. (2014). Assessing economically viable carbon reductions for the production of ammonia from biomass gasification. J. Clean. Prod. *64*, 581–589. https://doi.org/10.1016/j.jclepro.2013.09.011.

88. Bicer, Y., Dincer, I., Zamfirescu, C., Vezina, G., and Raso, F. (2016). Comparative life cycle assessment of various ammonia production methods. J. Clean. Prod. *135*, 1379–1395. https://doi.org/10.1016/j.jclepro.2016.07.023.

89. Pfromm, P.H. (2017). Towards sustainable agriculture: fossil-free ammonia. J. Renew. Sustain. Energy *9*, 034702. https://doi.org/10.1063/1.4985090.

90. Chen, J.G., Crooks, R.M., Seefeldt, L.C., Bren, K.L., Bullock, R.M., Darensbourg, M.Y., Holland, P.L., Hoffman, B., Janik, M.J., Jones, A.K., et al. (2018). Beyond fossil fuel–driven nitrogen transformations. Science *360*, eaar6611. https://doi.org/10.1126/science.aar6611.

91. MacFarlane, D.R., Cherepanov, P.V., Choi, J., Suryanto, B.H., Hodgetts, R.Y., Bakker, J.M., Ferrero Vallana, F.M., and Simonov, A.N. (2020). A roadmap to the ammonia economy. Joule *4*, 1186–1205. https://doi.org/10.1016/j.joule.2020.04.004.

92. Ghavam, S., Vahdati, M., Wilson, I.A.G., and Styring, P. (2021). Sustainable ammonia production processes. Front. Energy Res. *9*. https://doi.org/10.3389/fenrg.2021.580808.

93. Arora, P., Hoadley, A.F., Mahajani, S.M., and Ganesh, A. (2016). Small-scale ammonia production from biomass: a techno-enviro-economic perspective. Ind. Eng. Chem. Res. *55*, 6422–6434. https://doi.org/10.1021/acs.iecr.5b04937.

94. Ott, J., Gronemann, V., Pontzen, F., Fiedler, E., Grossmann, G., Kersebohm, D.B., Weiss, G., and Witte, C. (2012). Methanol. In Ullmann's Encyclopedia of Industrial Chemistry (Wiley-VCH Verlag GmbH & Co. KGaA). https://doi.org/10.1002/14356007.a16_465.pub3.

95. Mignard, D. (2003). Methanol synthesis from flue-gas $CO_2$ and renewable electricity: a feasibility study. Int. J. Hydrogen Energy *28*, 455–464. https://doi.org/10.1016/S0360-3199(02)00082-4.

96. Pontzen, F., Liebner, W., Gronemann, V., Rothaemel, M., and Ahlers, B. (2011). $CO_2$-based methanol and DME – efficient technologies for industrial scale production. Catal. Today *171*, 242–250. https://doi.org/10.1016/j.cattod.2011.04.049.

97. Van-Dal, É.S., and Bouallou, C. (2013). Design and simulation of a methanol production plant from $CO_2$ hydrogenation. J. Clean. Prod. *57*, 38–45. https://doi.org/10.1016/j.jclepro.2013.06.008.

98. Atsonios, K., Panopoulos, K.D., and Kakaras, E. (2016). Investigation of technical and economic aspects for methanol production through $CO_2$ hydrogenation. Int. J. Hydrogen Energy *41*, 2202–2214. https://doi.org/10.1016/j.ijhydene.2015.12.074.

99. Rivarolo, M., Bellotti, D., Magistri, L., and Massardo, A.F. (2016). Feasibility study of methanol production from different renewable sources and thermo-economic analysis. Int. J. Hydrogen Energy *41*, 2105–2116. https://doi.org/10.1016/j.ijhydene.2015.12.128.

100. 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. https://doi.org/10.1016/j.apenergy.2015.07.067.

101. 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. https://doi.org/10.1039/C9EE01673B.

102. Vázquez, D., and Guillén-Gosálbez, G. (2021). Process design within planetary boundaries: application to $CO_2$ based methanol production. Chem. Eng. Sci. *246*, 116891. https://doi.org/10.1016/j.ces.2021.116891.

103. Recycling International, C. (2022). Recycling $CO_2$ to Produce Methanol. https://www.carbonrecycling.is/co2-methanol.

104. Recycling International, C. (2022). World's Largest $CO_2$-to-methanol Plant Starts Production. https://www.carbonrecycling.is/news-media/worlds-largest-co2-to-methanol-plant-starts-production.

105. Hannula, I., and Kurkela, E. (2013). Liquid Transportation Fuels via Large-Scale Fluidisedbed Gasification of Lignocellulosic Biomass.

106. Zibunas, C., Meys, R., Kätelhön, A., and Bardow, A. (2022). Cost-optimal pathways towards net-zero chemicals and plastics based on a circular carbon economy. Comput. Chem. Eng. *162*, 107798. https://doi.org/10.1016/j.compchemeng.2022.107798.

107. Sutter, D., van der Spek, M., and Mazzotti, M. (2019). 110th anniversary : evaluation of $CO_2$ -based and $CO_2$ -free synthetic fuel systems using a net-zero-$CO_2$-emission framework. Ind. Eng. Chem. Res. *58*, 19958–19972. https://doi.org/10.1021/acs.iecr.9b00880.

108. Fasihi, M., Efimova, O., and Breyer, C. (2019). Techno-economic assessment of $CO_2$ direct air capture plants. J. Clean. Prod. *224*, 957–980. https://doi.org/10.1016/j.jclepro.2019.03.086.

109. Krekel, D., Samsun, R.C., Peters, R., and Stolten, D. (2018). The separation of $CO_2$ from ambient air – a techno-economic assessment. Appl. Energy *218*, 361–381. https://doi.org/10.1016/j.apenergy.2018.02.144.

110. 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. https://doi.org/10.1016/j.joule.2018.05.006.

111. González-Garay, A., Mac Dowell, N., and Shah, N. (2021). A carbon neutral chemical industry powered by the sun. Discov. Chem. Eng. *1*, 2. https://doi.org/10.1007/s43938-021-00002-x.

112. IEA (2019). The Future of Hydrogen.

113. Antonini, C., Treyer, K., Streb, A., van der Spek, M., Bauer, C., and Mazzotti, M. (2020). Hydrogen production from natural gas and biomethane with carbon capture and storage – a techno-environmental analysis. Sustain. Energy Fuels *4*, 2967–2986. https://doi.org/10.1039/D0SE00222D.

114. Antonini, C., Treyer, K., Moioli, E., Bauer, C., Schildhauer, T.J., and Mazzotti, M. (2021). Hydrogen from wood gasification with CCS – a techno-environmental analysis of production and use as transport fuel. Sustain. Energy Fuels *5*, 2602–2621. https://doi.org/10.1039/D0SE01637C.

115. van der Spek, M., Banet, C., Bauer, C., Gabrielli, P., Goldthorpe, W., Mazzotti, M., Munkejord, S.T., Røkke, N.A., Shah, N., Sunny, N., et al. (2022). Perspective on the hydrogen economy as a pathway to reach net-zero $CO_2$ emissions in Europe. Energy Environ. Sci. *15*, 1034–1077. https://doi.org/10.1039/D1EE02118D.

116. Bosch, R., van de Pol, M., and Philp, J. (2015). Policy: define biomass sustainability. Nature *523*, 526–527. https://doi.org/10.1038/523526a.

117. Rosa, L., Sanchez, D.L., and Mazzotti, M. (2021). Assessment of carbon dioxide removal potential via BECCS in a carbon-neutral Europe. Energy Environ. Sci. *14*, 3086–3097. https://doi.org/10.1039/D1EE00642H.

118. Sandalow, D., Aines, R., Friedmann, S.J., McCormick, C., and Sanchez, D.L. (2021). Biomass Carbon Removal and Storage (BiRCS) Roadmap.

119. D'Odorico, P., Davis, K.F., Rosa, L., Carr, J.A., Chiarelli, D., Dell'Angelo, J., Gephart, J., MacDonald, G.K., Seekell, D.A., Suweis, S., and Rulli, M.C. (2018). The global food-energy-water nexus. Rev. Geophys. *56*, 456–531. https://doi.org/10.1029/2017RG000591.

120. Sendi, M., Bui, M., Mac Dowell, N., and Fennell, P. (2022). Geospatial analysis of regional climate impacts to accelerate cost-efficient direct air capture deployment. One Earth *5*, 1153–1164. https://doi.org/10.1016/j.oneear.2022.09.003.

121. Becattini, V., Gabrielli, P., Antonini, C., Campos, J., Acquilino, A., Sansavini, G., and Mazzotti, M. (2022). Carbon dioxide capture, transport and storage supply chains: optimal economic and environmental performance of infrastructure rollout. Int. J. Greenh. Gas Control *117*, 103635. https://doi.org/10.1016/j.ijggc.2022.103635.

122. Gabrielli, P., Campos, J., Becattini, V., Mazzotti, M., and Sansavini, G. (2022). Optimization and assessment of carbon capture, transport and

storage supply chains for industrial sectors: the cost of resilience. Int. J. Greenh. Gas Control *121*, 103797. https://doi.org/10.1016/j.ijggc.2022.103797.

123. SaskPower. (2020). Boundary Dam Carbon Capture Project. https://www.saskpower.com/Our-Power-Future/Infrastructure-Projects/Carbon-Capture-and-Storage/Boundary-Dam-Carbon-Capture-Project.
124. NRG (2021). Petra Nova - carbon capture and the future of coal power. https://www.nrg.com/case-studies/petra-nova.html.
125. Equinor. (2019). Northern lights project concept report.
126. Snæbjörnsdóttir, S.Ó., Sigfússon, B., Marieni, C., Goldberg, D., Gislason, S.R., and Oelkers, E.H. (2020). Carbon dioxide storage through mineral carbonation. Nat. Rev. Earth Environ. *1*, 90–102. https://doi.org/10.1038/s43017-019-0011-8.
127. DemoUpCarma. (2022). DemoUpCarma & DemoUpStorage - the Project in Brief. http://www.demoupcarma.ethz.ch/en/home/.
128. Ringrose, P., Greenberg, S., Whittaker, S., Nazarian, B., and Oye, V. (2017). Building confidence in $CO_2$ storage using reference datasets from demonstration projects. Energy Proc. *114*, 3547–3557. https://doi.org/10.1016/j.egypro.2017.03.1484.
129. Ringrose, P.S. (2018). The CCS hub in Norway: some insights from 22 years of saline aquifer storage. Energy Proc. *146*, 166–172. https://doi.org/10.1016/j.egypro.2018.07.021.
130. Ringrose, P. (2020). How to Store $CO_2$ Underground: Insights from Early-Mover CCS Projects (Springer International Publishing). https://doi.org/10.1007/978-3-030-33113-9.
131. Abdulla, A., Hanna, R., Schell, K.R., Babacan, O., and Victor, D.G. (2021). Explaining successful and failed investments in U.S. carbon capture and storage using empirical and expert assessments. Environ. Res. Lett. *16*, 014036. https://doi.org/10.1088/1748-9326/abd19e.
132. Global CCS Institute (2021). Global Status of CCS 2021: CCS Accelerating to Net Zero. https://www.globalccsinstitute.com/resources/global-status-report/.
133. Zhang, Y., Jackson, C., and Krevor, S. (2022). An estimate of the amount of geological $CO_2$ storage over the period of 1996–2020. Environ. Sci. Technol. Lett. *9*, 693–698. https://doi.org/10.1021/acs.estlett.2c00296.
134. Broecks, K., Jack, C., ter Mors, E., Boomsma, C., and Shackley, S. (2021). How do people perceive carbon capture and storage for industrial processes? Examining factors underlying public opinion in The Netherlands and the United Kingdom. Energy Res. Social Sci. *81*, 102236. https://doi.org/10.1016/j.erss.2021.102236.
135. Lane, J., Greig, C., and Garnett, A. (2021). Uncertain storage prospects create a conundrum for carbon capture and storage ambitions. Nat. Clim. Change *11*, 925–936. https://doi.org/10.1038/s41558-021-01175-7.
136. Kearns, J., Teletzke, G., Palmer, J., Thomann, H., Kheshgi, H., Chen, Y.-H.H., Paltsev, S., and Herzog, H. (2017). Developing a consistent database for regional geologic $CO_2$ storage capacity worldwide. Energy Proc. *114*, 4697–4709. https://doi.org/10.1016/j.egypro.2017.03.1603.
137. Pale Blu Dot Energy (2020). Global Storage Resource Assessment – 2019 Update. https://www.globalccsinstitute.com/resources/publications-reports-research/global-storage-resource-assessment-2019-update/.
138. IEA (2021). The World Has Vast Capacity to Store $CO_2$: Net Zero Means We'll Need it.
139. 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. https://doi.org/10.1038/s41586-019-1681-6.
140. Ostovari, H., Sternberg, A., and Bardow, A. (2020). Rock 'n' use of $CO_2$: carbon footprint of carbon capture and utilization by mineralization. Sustain. Energy Fuels *4*, 4482–4496. https://doi.org/10.1039/D0SE00190B.
141. Ostovari, H., Müller, L., Mayer, F., and Bardow, A. (2022). A climate-optimal supply chain for $CO_2$ capture, utilization, and storage by mineralization. J. Clean. Prod. *360*, 131750. https://doi.org/10.1016/j.jclepro.2022.131750.
142. Tiefenthaler, J., Braune, L., Bauer, C., Sacchi, R., and Mazzotti, M. (2021). Technological demonstration and life cycle assessment of a negative emission value chain in the Swiss concrete sector. Front. Clim. *3*. https://doi.org/10.3389/fclim.2021.729259.
143. Rosa, L., Becattini, V., Gabrielli, P., Andreotti, A., and Mazzotti, M. (2022). Carbon dioxide mineralization in recycled concrete aggregates can contribute immediately to carbon-neutrality. Resour. Conserv. Recycl. *184*, 106436. https://doi.org/10.1016/j.resconrec.2022.106436.
144. Tanzer, S.E., and Ramírez, A. (2019). When are negative emissions negative emissions? Energy Environ. Sci. *12*, 1210–1218. https://doi.org/10.1039/C8EE03338B.
145. Becattini, V., Gabrielli, P., and Mazzotti, M. (2021). Role of carbon capture, storage, and utilization to enable a net-zero-$CO_2$ -emissions aviation sector. Ind. Eng. Chem. Res. *60*, 6848–6862. https://doi.org/10.1021/acs.iecr.0c05392.
146. Sunny, N., Bernardi, A., Danaci, D., Bui, M., Gonzalez-Garay, A., and Chachuat, B. (2022). A pathway towards net-zero emissions in oil refineries. Front. Chem. Eng. *4*. https://doi.org/10.3389/fceng.2022.804163.
147. Sternberg, A., and Bardow, A. (2015). Power-to-What? – Environmental assessment of energy storage systems. Energy Environ. Sci. *8*, 389–400. https://doi.org/10.1039/C4EE03051F.
148. Smith, P., Davis, S.J., Creutzig, F., Fuss, S., Minx, J., Gabrielle, B., Kato, E., Jackson, R.B., Cowie, A., Kriegler, E., et al. (2016). Biophysical and economic limits to negative $CO_2$emissions. Nat. Clim. Change *6*, 42–50. https://doi.org/10.1038/nclimate2870.
149. Nemet, G.F., Callaghan, M.W., Creutzig, F., Fuss, S., Hartmann, J., Hilaire, J., Lamb, W.F., Minx, J.C., Rogers, S., and Smith, P. (2018). Negative emissions—Part 3: innovation and upscaling. Environ. Res. Lett. *13*, 063003. https://doi.org/10.1088/1748-9326/aabff4.
150. United Nations Economic Commission for Europe (2022). Carbon Neutrality in the UNECE Region: Integrated Life-Cycle Assessment of Electricity Sources.
151. Rosa, L., Chiarelli, D.D., Rulli, M.C., Dell'Angelo, J., and D'Odorico, P. (2020). Global agricultural economic water scarcity. Sci. Adv. *6*, eaaz6031. https://doi.org/10.1126/sciadv.aaz6031.
152. Qiu, Y., Lamers, P., Daioglou, V., McQueen, N., de Boer, H.-S., Harmsen, M., Wilcox, J., Bardow, A., and Suh, S. (2022). Environmental trade-offs of direct air capture technologies in climate change mitigation toward 2100. Nat. Commun. *13*, 3635. https://doi.org/10.1038/s41467-022-31146-1.
153. Salah, C., Cobo, S., Pérez-Ramírez, J., and Guillén-Gosálbez, G. (2023). Environmental sustainability assessment of hydrogen from waste polymers. ACS Sustain. Chem. Eng. *11*, 3238–3247. https://doi.org/10.1021/acssuschemeng.2c05729.
154. Sultana, N., Hossain, S.M.Z., Aljameel, S.S., Omran, M.E., Razzak, S.A., Haq, B., and Hossain, M.M. (2023). Biohydrogen from food waste: modeling and estimation by machine learning based super learner approach. Int. J. Hydrogen Energy. https://doi.org/10.1016/j.ijhydene.2023.01.339.
155. Rosa, L., and Mazzotti, M. (2022). Potential for hydrogen production from sustainable biomass with carbon capture and storage. Renew. Sustain. Energy Rev. *157*, 112123. https://doi.org/10.1016/j.rser.2022.112123.
156. 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). Planetary boundaries: guiding human development on a changing planet. Science *80*, 347. https://doi.org/10.1126/science.1259855.
157. Wang-Erlandsson, L., Tobian, A., van der Ent, R.J., Fetzer, I., te Wierik, S., Porkka, M., Staal, A., Jaramillo, F., Dahlmann, H., Singh, C., et al. (2022). A planetary boundary for green water. Nat. Rev. Earth Environ. *3*, 380–392. https://doi.org/10.1038/s43017-022-00287-8.
158. Lambin, E.F., and Meyfroidt, P. (2011). Global land use change, economic globalization, and the looming land scarcity. Proc. Natl. Acad. Sci. USA *108*, 3465–3472. https://doi.org/10.1073/pnas.1100480108.
159. Slade, R., Bauen, A., and Gross, R. (2014). Global bioenergy resources. Nat. Clim. Change *4*, 99–105. https://doi.org/10.1038/nclimate2097.
160. Energy Transition Commission (2021). Bioresources within a Net-Zero Emissions Economy: Making a Sustainable Approach Possible. https://www.energy-transitions.org/publications/bioresources-within-a-net-zero-emissions-economy/.
161. Schyns, J.F., Hoekstra, A.Y., Booij, M.J., Hogeboom, R.J., and Mekonnen, M.M. (2019). Limits to the world's green water resources for food, feed, fiber, timber, and bioenergy. Proc. Natl. Acad. Sci. USA *116*, 4893–4898. https://doi.org/10.1073/pnas.1817380116.
162. Meldrum, J., Nettles-Anderson, S., Heath, G., and Macknick, J. (2013). Life cycle water use for electricity generation: a review and harmonization of literature estimates. Environ. Res. Lett. *8*, 015031. https://doi.org/10.1088/1748-9326/8/1/015031.
163. Tovar-Facio, J., Guerras, L.S., Ponce-Ortega, J.M., and Martín, M. (2021). Sustainable energy transition considering the water–energy nexus: a multiobjective optimization framework. ACS Sustain. Chem. Eng. *9*, 3768–3780. https://doi.org/10.1021/acssuschemeng.0c08694.

164. Rosa, L., Reimer, J.A., Went, M.S., and D'Odorico, P. (2020). Hydrological limits to carbon capture and storage. Nat. Sustain. *3*, 658–666. https://doi.org/10.1038/s41893-020-0532-7.

165. Sampson, G.S., Perry, E.D., and Tayler, M.R. (2020). The on-farm and near-farm effects of wind turbines on agricultural land values. J. Agric. Resour. Econ. *45*, 410–427. https://doi.org/10.22004/ag.econ.302463.

166. Barron-Gafford, G.A., Pavao-Zuckerman, M.A., Minor, R.L., Sutter, L.F., Barnett-Moreno, I., Blackett, D.T., Thompson, M., Dimond, K., Gerlak, A.K., Nabhan, G.P., and Macknick, J.E. (2019). Agrivoltaics provide mutual benefits across the food–energy–water nexus in drylands. Nat. Sustain. *2*, 848–855. https://doi.org/10.1038/s41893-019-0364-5.

167. Wang, S., Hausfather, Z., Davis, S., Lloyd, J., Olson, E.B., Liebermann, L., Núñez-Mujica, G.D., and McBride, J. (2023). Future demand for electricity generation materials under different climate mitigation scenarios. Joule *7*, 309–332. https://doi.org/10.1016/j.joule.2023.01.001.

168. Bang, Y.-Y., Hong, N.-J., Sung Lee, D., and Lim, S.-R. (2018). Comparative assessment of solar photovoltaic panels based on metal-derived hazardous waste, resource depletion, and toxicity potentials. Int. J. Green Energy *15*, 550–557. https://doi.org/10.1080/15435075.2018.1505618.

169. Moreau, V., Dos Reis, P., and Vuille, F. (2019). Enough metals? Resource constraints to supply a fully renewable energy system. Resources *8*, 29. https://doi.org/10.3390/resources8010029.

170. Reuters (2022). IEA Warns Global Solar Supply Chains Are Too Concentrated in China. https://www.reuters.com/business/energy/iea-warns-global-solar-supply-chains-are-too-concentrated-china-2022-07-07/.

171. Bunsen, J., Berger, M., and Finkbeiner, M. (2021). Planetary boundaries for water – a review. Ecol. Indicat. *121*, 107022. https://doi.org/10.1016/j.ecolind.2020.107022.

172. Tonelli, D., Rosa, L., Gabrielli, P., Caldeira, K., Parente, A., and Contino, F. (2023). Global Land and Water Limits to Electrolytic Hydrogen Production Using Wind and Solar Resources. Preprint. https://doi.org/10.21203/rs.3.rs-2724691/v1.

173. Wei, Y.-M., Kang, J.-N., Liu, L.-C., Li, Q., Wang, P.-T., Hou, J.-J., Liang, Q.-M., Liao, H., Huang, S.-F., and Yu, B. (2021). A proposed global layout of carbon capture and storage in line with a 2 °C climate target. Nat. Clim. Change *11*, 112–118. https://doi.org/10.1038/s41558-020-00960-0.

174. d'Amore, F., and Bezzo, F. (2017). Economic optimisation of European supply chains for $CO_2$ capture, transport and sequestration. Int. J. Greenh. Gas Control *65*, 99–116. https://doi.org/10.1016/j.ijggc.2017.08.015.

175. d'Amore, F., Sunny, N., Iruretagoyena, D., Bezzo, F., and Shah, N. (2019). European supply chains for carbon capture, transport and sequestration, with uncertainties in geological storage capacity: insights from economic optimisation. Comput. Chem. Eng. *129*, 106521. https://doi.org/10.1016/j.compchemeng.2019.106521.

176. Burger, J., Nöhl, J., Seiler, J., Gabrielli, P., Sansavini, G., and Bardow, A. (2022). Environmental impact of pioneering carbon capture, transport and storage chains. SSRN Electron. J. https://doi.org/10.2139/ssrn.4276719.

177. Azzaro-Pantel, C. (2018). Hydrogen Supply Chains (Elsevier). https://doi.org/10.1016/C2016-0-00605-8.

178. Shohan, S., Ali, S.M., Kabir, G., Ahmed, S.K., Suhi, S.A., and Haque, T. (2019). Green supply chain management in the chemical industry: structural framework of drivers. Int. J. Sustain. Dev. World Ecol. *26*, 752–768. https://doi.org/10.1080/13504509.2019.1674406.

179. Gabrielli, P., Charbonnier, F., Guidolin, A., and Mazzotti, M. (2020). Enabling low-carbon hydrogen supply chains through use of biomass and carbon capture and storage: a Swiss case study. Appl. Energy *275*, 115245. https://doi.org/10.1016/j.apenergy.2020.115245.

180. Luise, R., Brisse, A., and Azzaro-Pantel, C. (2021). Centralised vs. decentralised production and storage: optimal design of a decarbonised hydrogen supply chain with multiple end uses. In Computer Aided Chemical Engineering, *50*, pp. 1775–1780. https://doi.org/10.1016/B978-0-323-88506-5.50275-8.

181. Allen, C., Chuney, A., Halness, C., Jacobson, R., Kosar, U., and Suarez, V. (2022). Setting DAC on Track: Strategies for Hub Implementation.

182. Ishii, N., and Stuchtey, M. (2022). Planet Positive Chemicals: Pathways for the Chemical Industry to Enable a Sustainable Global Economy.

183. World Economic Forum (2022). Towards a Net-Zero Chemical Industry: A Global Policy Landscape for Low-Carbon Emitting Technologies.

184. Science Based Targets. (2022). Chemicals. https://sciencebasedtargets.org/sectors/chemicals.

185. Anderson, A., Lebling, K., Byrum, Z., and Dellesky, C. (2021). A New Industrial Revolution for a Livable Climate (World Resour. Inst). https://www.wri.org/insights/decarbonize-us-industry.

186. Chung, C., Kim, J., Sovacool, B.K., Griffiths, S., Bazilian, M., and Yang, M. (2023). Decarbonizing the chemical industry: a systematic review of sociotechnical systems, technological innovations, and policy options. Energy Res. Social Sci. *96*, 102955. https://doi.org/10.1016/j.erss.2023.102955.

187. Alexander, P., Brown, C., Arneth, A., Finnigan, J., Moran, D., and Rounsevell, M.D.A. (2017). Losses, inefficiencies and waste in the global food system. Agric. Syst. *153*, 190–200. https://doi.org/10.1016/j.agsy.2017.01.014.

188. Lassaletta, L., Billen, G., Grizzetti, B., Anglade, J., and Garnier, J. (2014). 50 year trends in nitrogen use efficiency of world cropping systems: the relationship between yield and nitrogen input to cropland. Environ. Res. Lett. *9*, 105011. https://doi.org/10.1088/1748-9326/9/10/105011.

189. Gao, Y., and Cabrera Serrenho, A. (2023). Greenhouse gas emissions from nitrogen fertilizers could be reduced by up to one-fifth of current levels by 2050 with combined interventions. Nat. Food *4*, 170–178. https://doi.org/10.1038/s43016-023-00698-w.

190. United Nations Environmental Assembly of the United Nations Environment Programme. (2022). Draft Resolution. End Plastic Pollution: Towards an International Legally Binding Instrument.

191. UK Department for Business, Energy and Industrial Strategy (2021). Biomass Feedstocks Innovation Programme (UK Department for Business, Energy and Industrial Strategy).

192. Wood, E. (2021). Federal Policies and Incentives Promoting Woody Biomass Production and Utilization.

193. Gabrielli, P., Gazzani, M., and Mazzotti, M. (2018). Electrochemical conversion technologies for optimal design of decentralized multi-energy systems: modeling framework and technology assessment. Appl. Energy *221*, 557–575. https://doi.org/10.1016/j.apenergy.2018.03.149.

194. Abanades, J.C., Rubin, E.S., Mazzotti, M., and Herzog, H.J. (2017). On the climate change mitigation potential of $CO_2$ conversion to fuels. Energy Environ. Sci. *10*, 2491–2499. https://doi.org/10.1039/C7EE02819A.

195. R&D Dep (2019). CASALE. https://www.casale.ch/.

196. Gabrielli, P., Acquilino, A., Siri, S., Bracco, S., Sansavini, G., and Mazzotti, M. (2020). Optimization of low-carbon multi-energy systems with seasonal geothermal energy storage: the Anergy Grid of ETH Zurich. Energy Convers. Manag. X *8*, 100052. https://doi.org/10.1016/j.ecmx.2020.100052.

197. International Fertilizer Association (IFA) (2022). IFASTAT Database. https://www.ifastat.org/.

198. Statista. (2022). Statista Database. https://www.statista.com/.

199. Mekonnen, M.M., and Hoekstra, A.Y. (2016). Four billion people facing severe water scarcity. Sci. Adv. *2*, e1500323. https://doi.org/10.1126/sciadv.1500323.

200. Food and Agriculture Organization of the United Nations (FAO) (2022). FAOSTAT Database. https://www.fao.org/faostat/en/.

201. Food and Agriculture Organization of the United Nations (FAO) (2022). AQUASTAT Database. https://www.fao.org/aquastat/statistics/query/index.html?lang=en.

202. Vanham, D., Alfieri, L., Flörke, M., Grimaldi, S., Lorini, V., de Roo, A., and Feyen, L. (2021). The number of people exposed to water stress in relation to how much water is reserved for the environment: a global modelling study. Lancet Planet. Health *5*, e766–e774. https://doi.org/10.1016/S2542-5196(21)00234-5.