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Technological and policy options for the defossilisation of chemical manufacturing†

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The chemical industry plays a pivotal role in modern society, providing essential products like plastics, consumer products, pharmaceuticals, speciality and agricultural chemicals. With increasing global prosperity and evolving societal demands, the need for sustainable chemicals is more pressing than ever. Essentially, the production of chemicals as we know it today is based on the use of fossil fuel for supplying the feedstock needed to provide the carbon-skeleton and the energy required for the synthesis process. As either of the two leads to CO₂ emissions, net-zero in chemistry requires both renewable energy and sustainable carbon supply strategies. Decarbonisation in the chemical industry requires the use of carbon-free renewable energy and changes in process design to replace CO₂ liberating steps (mainly energy supply) during manufacturing, e.g. with hydrogen as a reducing agent. While defossilisation technologies refer to using defossilised carbon feedstock for material production, namely biomass, or carbon supplied via carbon capture and utilisation (CCU) or from recycling of carbonaceous waste streams. This paper presents a meta-analysis of net-zero transition scenarios for the chemical industry to achieve net-zero emissions by 2050, focusing on feedstock structures and renewable energy requirements. Additionally, it evaluates the sustainability of defossilisation technologies and underscores the imperative of target-oriented cooperation of industry, policymakers, academia, and the public to facilitate a rapid transition towards a more sustainable chemical industry.

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Sustainability spotlight

This study critically examines how the transition to sustainable feedstocks – such as biomass, recyclates, or captured CO₂ – can steer ammonia, organic chemical and plastics manufacturing toward net-zero emissions by 2050. We analyse the aspects of net-zero transition scenarios, focusing on projected future chemical demand, feedstock sources, and renewable energy requirements for assessing the sustainability of key defossilisation technologies across environmental, social, and economic dimensions. With the generated insights, we seek to contribute to shaping a practical net-zero roadmap, underpinning the industry's alignment with the UN Sustainable Development Goals 7 (affordable and clean energy), 9 (industry, innovation and infrastructure), 12 (responsible consumption and production), and 13 (climate action).

1. Introduction

Organic chemistry is one of the important drivers for the emergence of the Second Industrial Revolution. In the meantime, products generated by the art of chemistry find applications in virtually any industry sector yielding products including but not limited to plastics, consumer goods, lubricants, adhesives, healthcare products, and agrochemicals. It's as simple as that – no modern life without chemistry. Scarcity of resources, energy crisis, supply chain issues, environmental degradation, and most importantly the need to minimise greenhouse gas

(GHG) emissions have raised the interest in strengthening supply chain diversification, local industrial resilience, nature conservation, and above all in the transformation towards a net-zero chemical industry. Of note, net-zero does not mean zero emissions, but rather that the amount of GHG emitted is balanced by active removal and sequestration of a similar amount from the atmosphere or from process or incineration gases.

Emissions generally accrue at three different stages (Fig. 1): scope 1 emissions are directly caused by sources owned or controlled by the manufacturing firm; scope 2 are indirect emissions attributed to the purchase of electric power or process heat, while scope 3 are indirect emissions that result from the activity of a firm but are not under their direct control. Scope 3 emissions are further divided into upstream emissions encompassing emissions resulting from the production of purchased raw materials and services (including raw material extraction and transportation), and downstream emissions

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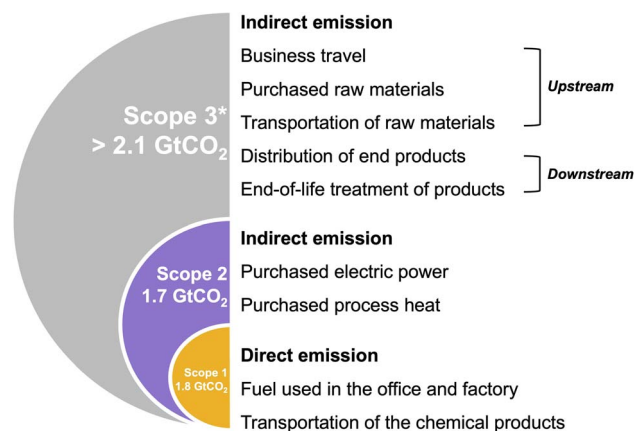


Fig. 1 Scope 1, 2, 3 greenhouse gas emissions of the chemical industry in 2021. *Scope 3 upstream emissions were 2.1 Gt while downstream emissions are not accounted for here.¹ The list of scope 3 emissions here is not exhaustive.²

including distribution of finished products, product use and end-of-life (EOL) treatment of the manufactured goods.^{3,4} In fact, scope 1 and 2 GHG emissions of the chemical industry are considerable, amounting to 6% of global emissions (3.5 Gt CO₂ eq. out of 59 Gt CO₂ eq.). Assessment of scope 3 emissions is notoriously difficult, as it requires emission data input from suppliers, producers, distributors, users as well as from facilities disposing, treating and processing waste. Downstream emissions, in particular, are challenging to track and are not included here due to methodological difficulties and huge data variations.⁴ Nevertheless, recent published work indicated scope 3 upstream emissions may add up more than 50% of the already accounted for GHG emissions (Fig. 1).¹ This suggests that the total emissions from the chemical industry could indeed exceed 5.6 Gt CO₂ eq. hence representing nearly 10% of the total global CO₂ emissions.^{1,5}

While reducing a considerable fraction of scope 1 and 2 emissions is possible by adopting alternative organisational routines, using renewable instead of fossil-based utilities or optimising logistics, abating scope 3 is challenging. The essential reason is that most organic primary chemical (see ESI Appendix†) products are composed to a considerable extent (>80% w/w) of carbon currently predominately derived from the geosphere in the form of oil, gas, and coal. In addition to fossil-based GHG emissions accruing upstream during feedstock mining, transportation and transformation, at the EOL of the manufactured chemical or chemicals-containing products, vast amounts of carbon previously safely stowed away underground are released in the course of incineration, biological or chemical degradation (e.g. in the sewage treatment plants). If not captured and sequestered, these gaseous carbonaceous (CO₂, CO, methane) GHG waste stream are subsequently released into the atmosphere. As the resulting carbon chain is linear, carbon from the geosphere is hence continuously carried over into the atmosphere thereby significantly contributing to global greenhouse gas emissions.

In alignment with the Paris Agreement to limit global warming to 1.5 °C by the end of this century, CO₂ emissions should reach net-zero by 2050 in any larger geopolitical area.⁶ For example, China, as the largest emitter of GHG in the world, has planned to reach peak CO₂ emissions by 2030 and is committed to achieving carbon neutrality by 2060 through implemented policies, including a national emissions trading system and investments in renewable energy.⁷ The European Union is acting under its European Green Deal, aiming GHG emissions be 55% lower in 2030 compared to 1990,⁸ meanwhile the European Commission acknowledges electrification and hydrogen as key technologies.^{9,10} Furthermore, the global drive to use non-fossil based fuels in the transport sector (renewable fuels of non-biological origin or RFNBO, recycled carbon fuels or RCF, and sustainable aviation fuel or SAF) are pillars recognised to contribute to the deployment of net-zero technologies for supply of redox-reduced carbon though predominately for energetic applications and not as feedstock.^{11,12}

On the international level, the chemical industry is sharing the 1.5 °C goal and has to work on reducing its CO₂ emissions to achieve net-zero by 2050. For the chemical industry, defossilisation, *i.e.* the replacement of fossil-based feedstocks with alternative, non-fossil sources of carbon for product manufacturing, provides a promising avenue for reaching net-zero emission (Fig. 2). Notably, defossilisation is also a crucial concept in the context of the Science Based Targets initiative (SBTi), which aims to support companies in setting targets to reduce their GHG emissions and limit global warming. SBTi recognises the importance of defossilisation and encourages companies to develop strategies that align with a low-carbon, sustainable future.⁴

Several emerging technologies for sustainable chemical production are already being recognised and implemented to enhance efficiency, reduce energy consumption, and lower environmental impacts. For example, (a) biotransformation,^{13–15} which utilises biological systems such as enzymes or microorganisms to catalyse reactions under mild conditions using renewable feedstocks like biomass; (b) flow chemistry,¹⁶ which improves reaction control and efficiency through continuous flow systems, leading to reduced energy use and byproducts; (c) photochemistry,¹⁷ which leverages light to drive reactions under mild conditions, with the potential to use renewable energy sources like sunlight and (d) water-based chemistry,^{18,19} which substitutes harmful solvents with water, reducing environmental impact and enhancing safety. These technologies reduce reliance on fossil fuels while promoting circularity and resource efficiency. Our study focuses on the broader impacts of these technologies on bulk chemical production and feedstock transformations, without delving into detailed technical aspects.

Another notable trend is product innovation at the chemical and polymer level. For instance, biogenic carbon (e.g. furandicarboxylic acid (FDCA) by Avantium,²⁰ Glycix by Plantics,²¹ Velvetol® by WeylChem²²) is increasingly being used for the production of polymers with significantly higher oxygen but lower energy and carbon content if compared to conventional polymers like polyethylene, polypropylene or polystyrene. This shift is expected to result in substantial reductions in carbon



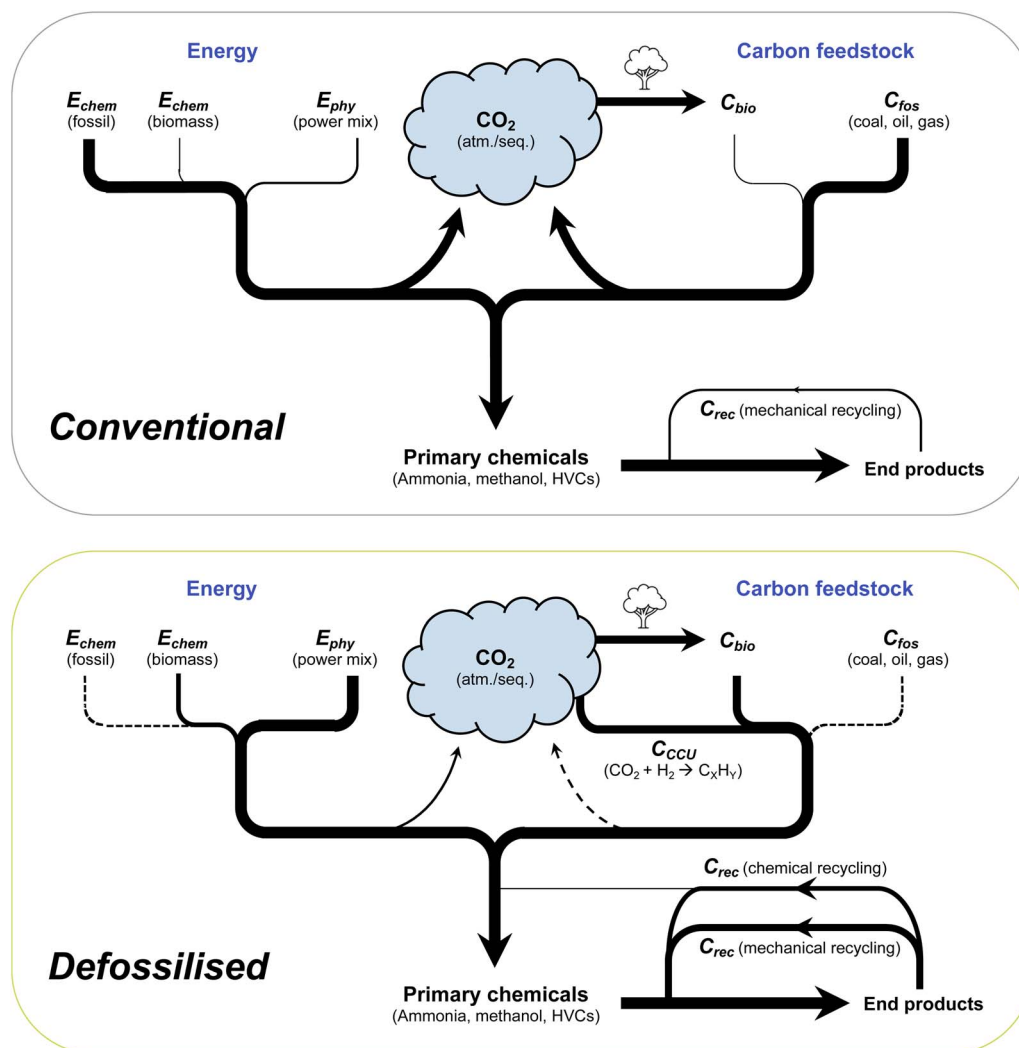


Fig. 2 Material and energy flow of the chemical industry today and once defossilised. Today, carbon feedstock is sourced from fossil fuels (coal, oil, gas) with a small fraction (less than 1%) of biomass and recycled plastics (9%) added. Similarly, energy is predominantly derived from fossil fuels. In a defossilised scenario, larger fractions of feedstock are generated by carbon capture and utilisation (CO_2 from unavoidable exhaust gases or from the atmosphere), or obtained from biomass, or massive recycling of plastics. The share of fossil fuels is hence decreased, and residual CO_2 emissions are captured and stored (CCS). While this process does not fully achieve defossilisation, it is included here as part of the low-carbon emission scenarios discussed in our analysis. Energy is then predominantly obtained from biomass or carbon-free electricity generated from renewables. In all of the analysed scenarios, a product mix of primary chemicals (ammonia, methanol, and high value chemicals, including ethylene, propylene, benzene, toluene, and mixed xylenes), which are then transformed into the various industrial, professional, or consumer end products but also used energetically in the transport and agricultural sector are manufactured. The thickness of the arrows shall indicate the relative size of the energy or carbon streams. Dotted arrows indicate the continued use of fossil fuels coupled with CCS, a practical option to reach a net-zero chemical industry, although it is not considered a defossilisation technology.

emissions.²³ We believe, we are in a phase where innovation is not only focused on improving the processes used to produce standard plastics, but also on developing entirely new precursors and polymers with an inherently lower environmental footprint – especially when derived from defossilised feedstocks.

In 2020, 160 PWh of primary energy was produced and consumed globally, with 79% from fossil carbon, 5% from nuclear, and 16% from renewables.²⁴ Of this, 13 PWh of fossil fuels was directed to the chemical industry meeting over 99% of its energy and carbon feedstock needs.²⁵ For defossilisation of the chemical industry (Fig. 2) both energy and carbon feedstock supply have to be rewired. While energy (electricity and heat) can be obtained

from renewables (e.g. solar, wind, hydrodynamics, or biomass), carbonaceous feedstock input will have to be defossilised, i.e. of non-fossil origin. For the supply of non-fossil origin carbon, only two paths are known: first, recycles. While recycled carbon might indeed be of fossil origin, its reuse allows a reduction of additional virgin carbon input. As long as this input originates from non-fossil sources, CO_2 emissions are subsequently decreased throughout the entire value-added chain. Second, atmospheric carbon.²⁶ CO_2 can either be captured from concentrated point source emitters (PS), directly from air (DAC), or by plants. In subsequent steps, this carbon can then either be used directly or redox reduced with hydrogen to give defossilised feedstock.



Noteworthy, some CO₂ emissions can alternatively be reduced further if the carbon released at the end of the product's lifecycle is captured and stored (CCS†) underground for geological periods. To this end, CCS has high potential to contribute to reducing CO₂ emissions of the chemical industry but is in itself not a defossilisation technology as fossil carbon input is still permissive. Notably, enabling a defossilised net-zero chemical industry requires careful balancing of material and emission streams and energy demand. As huge capital investments are required to achieve the turnaround, policy measures are required to promote efforts towards net-zero chemistry. However, this requires a better understanding of the interrelationships described here among the political players, who already find themselves in an increasingly complex setting. We are obviously aware that CCS can also be combined with biomass utilisation (BIO) and carbon capture and utilisation (CCU) or CCU can be combined with recycling.²⁷ However, taking such combinations into account would only unnecessarily complicate our considerations and hardly provide any additional gain in accuracy – in a situation in which the forecasts are already subject to quite some inaccuracies.

Interestingly, the results of net-zero transition scenarios which consider the transition to a close CO₂-neutral or CO₂-neutral chemistry^{28–34} found in the public domain vary considerably. As outlined in here, this variation is at least in part due to different assumptions regarding the chemicals involved, emissions scopes, the mix of technologies used and the energy requirements. For non-specialists, including most policy-makers, it's hence difficult to determine the path forward. One of the goals of this study is to analyse the space of possibilities as represented by a selected number of peer-reviewed net-zero transition scenarios and to distil a number of generic rules.

We have also analysed the influence of the different technology paths at a higher, more abstract level. This analysis is based on the three-pillar model of sustainability. We rated the technological options according to a greatly simplified evaluation scheme, whereby the three pillars of sustainability were broken down into components that are relevant in the context of net-zero chemistry. The main aim is to work out the impact of the deployment of the proposed technologies on society, economy and environment. This was done in order to provide an arbitrate metric for sustainability measurement beyond the scope of climate effects.

2. Analysis of net-zero transition scenarios

2.1. Background and objectives

In the meta-analysis presented here, the net-zero transition scenarios from the scientific publications were selected based on the following criteria:

- (a) Focus on the global chemical industry.

- (b) Published no later than 2018.

- (c) Shift from fossil-based to partially or completely defossilised feedstock.

- (d) Provision of quantitative data on carbon feedstock input and energy consumption for the production of primary chemicals.

- (e) Demonstration of net-zero or near-net-zero CO₂ emissions.

In total seven net-zero transition scenarios presented in five publications were selected (Table 1) outlining development paths until 2050 and 2030, respectively. When multiple scenarios were reported, we selected one or two for our analysis based on the following rationale. From Meng *et al.*,²⁹ LC-NFAX and HC-NFAX both display the highest fossil fuel reduction rates combined with two different circularity strategies. Scenario NZE2050H from Lopez *et al.*³⁰ is based on maximising biomass input. From Katelhon's work,³² TRLH features a high technology readiness level. Our selection of the net-zero transition scenarios aims to provide a non-biased and broad scope.

All authors focused on the production of primary chemicals, *i.e.* ammonia and methanol and high-value chemicals (HVCs including ethylene, propylene, benzene, toluene, and mixed xylenes, see also ESI Appendix†). Curiously, all studies extrapolated key data (*e.g.* the future chemical demand and recycling quotes) from one of two reports of the International Energy Agency (IEA) published in 2013 and 2018 (ref. 37 and 38) prior to making scenario-specific modifications. Feedstock was primarily sourced from fossil reserves but generally combined with CCS (FOS/CCS), CCU with CO₂ obtained from point source emitters or ambient air, biomass (BIO), or recycling of plastic waste (REC). ZERO1.5, LC-NFAX/HC-NFAX and EmiL anticipate additional capacities for ammonia and methanol production, targeting use in the energy and transport sector.^{35,36} ZERO1.5, LC-NFAX/HC-NFAX, NZE2050H and EmiL assume elevated plastic collection and recycling rates of 18% in the 2018 IEA report.³⁷

On the energy side, ZERO1.5, LC-NFAX/HC-NFAX, and EmiH/EmiL considered only the demand for conversion of feedstock into primary chemicals, while NZE2050H and TRLH, also accounted for their conversion into large-volume secondary chemicals (polyethylene, vinyl chloride, ethylene oxide, styrene, polypropylene, acrylonitrile, propylene oxide, acetone, phenol, terephthalic acid, *para*-xylene, caprolactam, cumene, diethylene glycol, ethylene glycol).

All authors assumed unlimited availability of net-zero energy for power and heat production, as well as for the supply and transport of carbon (biomass, fossil fuels, or CO₂). EOL emissions were generally considered, assuming incineration or landfill as the means for the removal of a fraction of product-bound carbon (LC-NFAX/HC-NFAX).

We first set out to harmonise the data, aiming to estimate (a) the projected future demand for primary chemicals; (b) the proposed virgin feedstock cocktails; (c) the demand for renewable electricity. In this way, we sought to outline the realm of possibilities potentially enabling net-zero emission chemistry.

† We are obviously aware that CCS can also be combined with BIO and CCU. However, taking such combinations into account would only unnecessarily complicate our considerations and hardly provide any additional gain in accuracy – in a situation in which the forecasts are already subject to quite some inaccuracies.



Table 1 Net-zero transition scenarios demonstrating zero emission of the chemical industry by 2050^a

Publications	Deployed technologies					Energy demand ^c	
	FOS/CCS	CCU	BIO	Scaling of cross-sector applications	Recycling intensification	Primary	Secondary
ZERO1.5 ²⁸	X	X	X	X	X	X	
LC-NFAX ²⁹	X	X	X	X	X	X	
HC-NFAX ²⁹	X	X	X	X	X	X	
NZE2050H ³⁰		X	X		X		X
EmiH ³¹		X				X	
EmiL ³¹		X		X	X	X	
TRLH ^{32/b}		X					X

^a ZERO1.5 (ref. 28) – techno-economical assessment of 20 decarbonisation approaches. LC-NFAX/HC-NFAX²⁹ – modesty-driven scenario (see next section; low circularity/high circularity, LC/HC) assuming dwindling demands of chemical consumption due to regulations and a change of consumer habits. NZE2050H³⁰ – maximisation of the use of sustainably produced biomass as feedstock, with feedstock supply gaps filled by CO₂ captured from the gas phase. EmiH/EmiL³¹ – all feedstock for chemical production is supplied by unavoidable CO₂ emissions accruing in the course of steel and cement production. TRLH³² – an aggressive scenario assuming the transition of the chemical industry by 2030 to reach net-zero deploying high technology readiness level technologies (TRL >7). FOS/CCS: fossil feedstock combined with carbon capture and storage; CCU: carbon capture and utilisation; BIO: biomass utilisation; Scaling of cross-sector applications: massive increase of ammonia and methanol production volumes for application as fuel in the transport and energy sector.^{35,36} Recycling intensification: recycling rates considerably exceed the 18% proposed by IEA.³⁷ ^b Demonstrates net-zero until 2030. ^c Primary: only the energy expenses required for converting feedstock into primary chemicals are considered. Secondary: energy required for conversion of primary into secondary chemicals (polyethylene, vinyl chloride, ethylene oxide, styrene, polypropylene, acrylonitrile, propylene oxide, acetone, phenol, terephthalic acid, *para*-xylene, caprolactam, cumene, diethylene glycol, ethylene glycol) is also considered. The additional energy requirements account for less than 5% of the total feedstock input³⁰ and were therefore neglected by us.

2.2. Projected production volumes, carbon flow and energy content for primary chemical manufacturing

For projection of the future primary chemicals demand, all net-zero transition scenarios used input data from IEA published in 2013 (NZE2050H, TRLH) and 2018 (ZERO1.5, LC-NFAX, HC-NFAX, EmiH, EmiL) predicting a demand of 1380 Mt and 1001 Mt, respectively.^{37,38} IEA calculated those demands based on economic parameters such as country/regional data of the gross domestic product (GDP), disposable income, short-term industrial capacities, current materials consumptions, demand saturation levels derived from historical demand intensity curves, resource endowments, and the fraction of feedstock being recycled from plastic waste.³⁷

IEA demand projections were then further modified by the authors of the net-zero transition scenarios first considering (a) the impact of the reduction of chemical demand through eliminating, reusing and substituting with non-carbon-based alternatives; then (b) scaling of cross-sector applications with increased demand of ammonia and methanol, and lastly; (c) reduction of *de novo* synthesised chemicals due to plastic recycling.

ZERO1.5 (Fig. 3A–C) projects chemical production of 1275 Mt (484 MtC) and an additional 279 Mt (237 MtC) obtained from recycled plastics assuming an exceptionally high recycling rate of 66%. Consequently, HVCs production volumes are considered to grow at a CAGR of 0.9% (453 Mt/398 MtC) falling significantly below the 2.4% proposed by IEA (580 Mt/506 MtC).³⁷ Due to the proposed massive future use of ammonia (598 Mt) and methanol (224 Mt/84 MtC) as chemical energy carriers, the projected production volumes exceed those proposed by IEA (ammonia 241 Mt and methanol 180 Mt) by a factor of 2.5 and 1.2, respectively. The overall energy embedded in the produced chemicals amounts to 9.9 PWh, with 3.1 PWh in ammonia, 1.2 PWh in methanol and 5.6 PWh in HVCs.

LC-NFAX and HC-NFAX scenarios propose a primary chemical demand of 1760 Mt thereby considerably exceeding the IEA prognosis of 972 Mt, mainly due to cross-sector applications in marine transport and power balancing. The authors propose an aggressive circularity strategy (including eliminating, reusing, and substituting) and assume high plastic recycling rates (37% in LC-NFAX and 43% in HC-NFAX). To this end, the demand for newly synthesised HVC is reduced by 98 Mt (89 MtC, see also ref. 25) and 101 Mt (92 MtC) to give HVC production volumes of 330 Mt (288 MtC) and 221 Mt (193 MtC). While the authors proposed an increase of ammonia volumes (LC-NFAX 996 Mt; HC-NFAX 968 Mt) for transport and energetic use, methanol production volumes are considered to decrease to (LC-NFAX 74 Mt/28 MtC, HC-NFAX 62 Mt/23 MtC) assuming no future use as engine fuel. The resulting *de novo* synthesised chemicals hence amounted to 1400 Mt and 1251 Mt for LC-NFAX and HC-NFAX, respectively. The total energy embedded in *de novo* synthesised chemicals in LC-NFAX was 9.7 PWh, with 5.2 PWh in ammonia, 0.4 PWh in methanol and 4.1 PWh in HVCs; in HC-NFAX, decrease of HVC production leads to a reduction of total energy for *de novo* synthesised chemicals to 8.3 PWh, with 5.1 PWh in ammonia, 0.3 PWh in methanol and 2.8 PWh in HVCs.

NZE2050H projects a total chemical demand of 1538 Mt (958 MtC) in 2050. A 60% plastics recycling rate leads to 224 Mt (190 MtC) recycling materials while the *de novo* synthesised chemicals amounting to 1314 Mt (768 MtC). HVCs demand is expected to see a significant upsurge to 785 Mt (689 MtC). Ammonia and methanol production are expected to steadily rise to 317 Mt and 212 Mt (79 MtC), respectively. A total of 12.5 PWh of energy is embedded in *de novo* synthesised chemicals, with 1.7 PWh in ammonia, 1.2 PWh in methanol, and 9.7 PWh in HVCs.



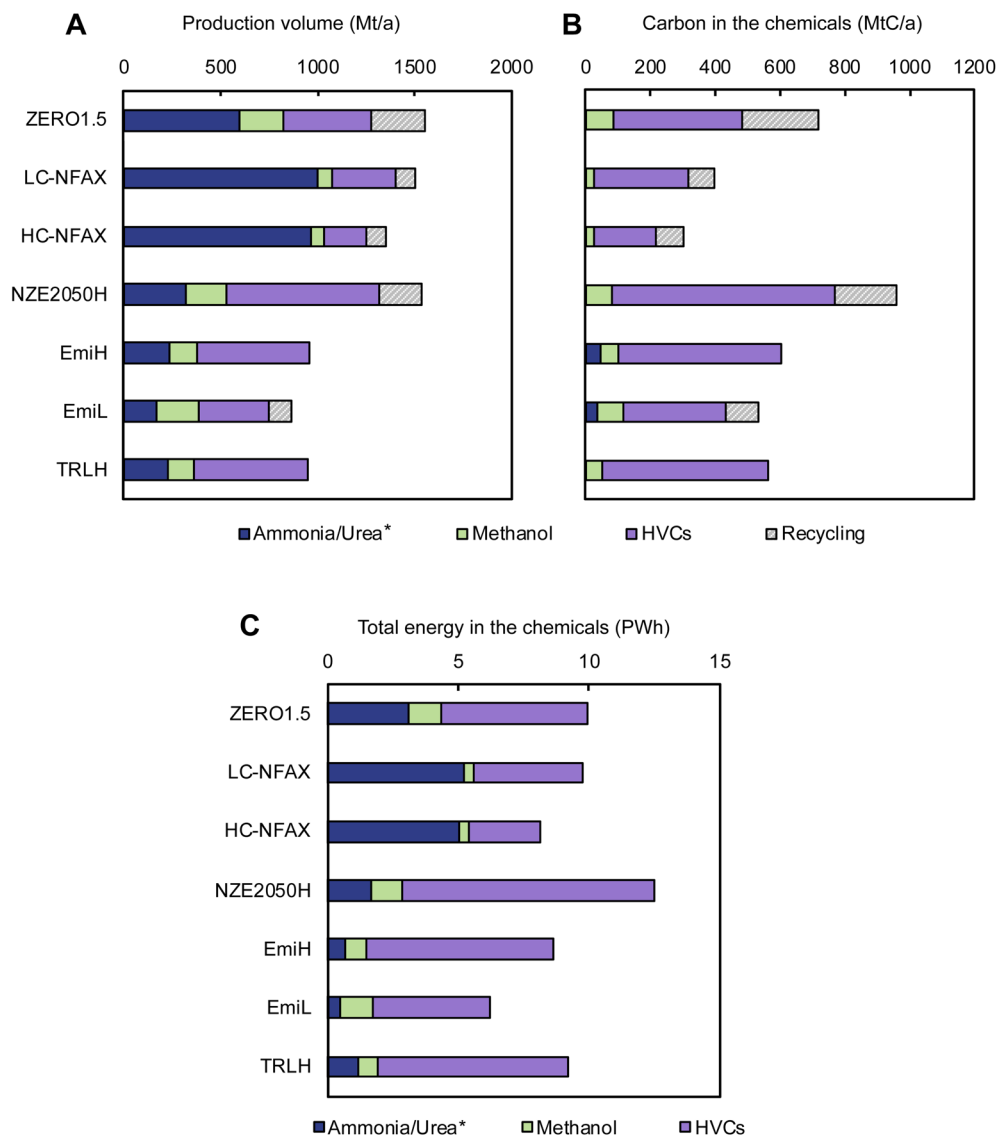


Fig. 3 Projected mass and energy content of chemical demand in net-zero transition scenarios. Projected demand for chemicals in (A) metric tons and (B) metric tons of carbon. (C) Total chemical energy embedded in *de novo* synthesised chemicals (recycled chemicals excluded) expressed in lower heating values. Methanol converted to HVCs has been subtracted to prevent double counting. By-products, such as C4 chemicals (butadiene, butylene), of ethylene manufacturing and cracking of fossil reserves^{39,40} are neglected. *Generally, ammonia equivalents except for EmiH and EmiL stating urea production volumes and energy.

For calculation of the future chemical demand in EmiH, the IEA data were transferred directly projecting 953 Mt in 2050. Of note, the authors proposed production of massive amounts of urea and its application as fertiliser. In EmiL, primary chemical demand was reduced to 862 Mt (532 MtC), assembled from 751 Mt (433 MtC) of *de novo* synthesised and 111 Mt (99 MtC) of recycled materials. Urea is expected to encounter negative growth to 165 Mt (33 MtC) by 2050 due to reduced nitrogen fertiliser use.⁴¹ Methanol is projected to grow faster as in the IEA scenario to 224 Mt²⁸ due to its use in transportation, while HVCs demand are reduced by 45% to 362 Mt (316 MtC) due to reuse and recycling.⁴² In EmiH, a total of 8.6 PWh of energy is embedded in *de novo* synthesised chemicals, with 0.7 PWh in urea, 0.8 PWh in methanol, and 7.2 PWh in HVCs. In EmiL, the

total embedded energy is 6.2 PWh, with 0.5 PWh in urea, 1.2 PWh in methanol, and 4.5 PWh in HVCs.

In TRLH, again the IEA data were used unchanged assuming production of 948 Mt (562 MtC) of primary chemicals by 2030. The production volumes for ammonia, methanol and HVCs are 229 Mt, 135 Mt (51 MtC) and 584 Mt (511 MtC), respectively. The total embedded energy in *de novo* synthesised chemicals is 9.2 PWh, with 1.2 PWh in ammonia, 0.7 PWh in methanol, and 7.2 PWh in HVCs.

Consequently, the 2050 production data in the net-zero transition scenarios differ from each other (751 Mt to 1418 Mt, Fig. 3A) and, in most cases, fall short of the referenced baseline scenarios (IEA 2013: 1380 Mt and 2018: 1001 Mt, because of assumptions of reasonable and informed customer



behaviour and policies. Of note, IPCC dealing with global carbon fluxes too, relies on more dynamic datasets and standardised narratives in order to size those potential non-linear changes.⁴³ We argue that standardisation of the input data used for net-zero scenario development would further increase data transparency.

Scaling of ammonia and methanol for cross-sector applications and recycling intensification also contribute to the significant variations in the material flows. Particularly, ammonia production in LC-NFAX and HC-NFAX, accounting for two-thirds of the total production volume, adds complexity to the system. Since ammonia contains no carbon and has the lowest energy content of all primary chemicals, producing ammonia would require the least energy and could be decarbonised. On the other hand, intensified recycling mainly leads to reduced burden from HVCs production due to their high carbon and chemical energy content (see Fig. S1†) thereby also translating into lower energy input. Production volumes in HC-NFAX (lowest HVCs demand of 221 Mt) and NZE2050H (highest HVC demand of 785 Mt) differ by a factor of three while the carbon and energy-flow are similar (1264 Mt and 1314 Mt). As the gap is filled by ammonia carrying comparatively low chemical energy and being void of carbon, a considerable amount of both, carbon and energy, will have to be accounted for in HC-NFAX if circularity and modesty measures fail.

The total chemical energy in *de novo* synthesised chemicals ranges from 6.2 to 11.0 PWh (Fig. 3C). As said, the majority of the chemical energy is in HVCs. Therefore, plastics, comprising 24% of the total chemical output⁴⁴ and primarily sourced from HVCs, are crucial for reducing energy input through recycling.

Regardless of the production volume for each primary chemical and as a whole, the weighted average energy content of the *de novo* synthesised chemicals falls within 6.6 to 9.7 TWh per Mt (Fig. S2†), indicating a benchmark for the energy input for production.

2.3. Supply of virgin carbon as feedstock

The virgin carbon feedstock required for the build-up of *de novo* synthesised chemicals is analysed in the following section (Fig. 4).

In the ZERO1.5 scenario, fossil inputs account for 39% (494 MtC), biomass for 43% (545 MtC), and CCU for 18% (226 Mt). In LC-NFAX and HC-NFAX, fossil inputs account for 18% and 25% (77 MtC and 73 MtC), biomass for 44% and 45% (188 MtC and 131 MtC), and CCU for 37% and 30% (158 MtC and 89 MtC) of the carbon input, respectively. Additionally, 11 MtC from plastic pyrolysis was added but neglected by us for simplification. In the NZE2050H scenario, 51% of the carbon is sourced from biomass, amounting to 1108 MtC, while 49% is sourced from CCU, equating to 1083 MtC.

EmiH and EmiL investigated the feasibility of fully relying on CO₂ as its carbon source in 2050, where 845 MtC and 600 MtC in the form of CO₂ would be used in *de novo* synthesised chemicals production sourced from large point source emitters (power, cement, steel, pulp and paper sectors). Likewise, CO₂ is envisioned to serve as the sole carbon source for chemical production by 2030 in TRLH, equivalent to 1014 MtC.

The utilisation of biomass in net-zero transition scenarios varies by almost a factor of eight (131 to 1108 MtC across ZERO1.5, LC-NFAX, HC-NFAX, NZE2050H, Fig. 4), with all authors projecting significantly increased consumption compared to less than 1% as of today. Clearly, biomass as feedstock has the advantage that it not only provides carbon but also chemical energy (Fig. S1†). Still, its use must be carefully balanced with food and crop production, direct energy use, and other material applications.⁴⁵ CO₂, on the other hand, is vastly abundant and adds considerably to the feedstock mix in EmiH, EmiL and TRLH. However, as we did not analyse the data with regard to the fraction of carbon removed from the scenarios by CCS, we cannot challenge the data but want to remind the reader that the CCS

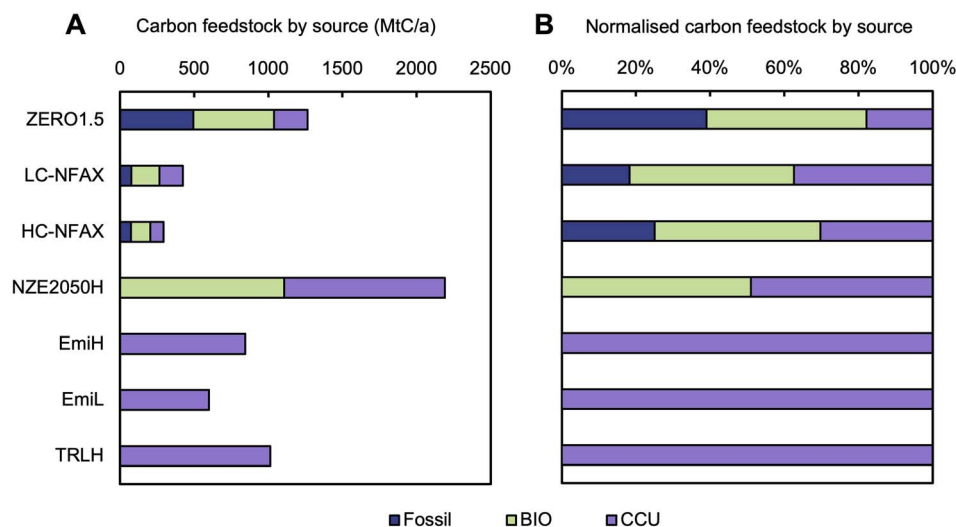


Fig. 4 Virgin carbon feedstock input for chemical production in net-zero transition scenarios. (A) Carbon feedstock by source. (B) Normalised carbon feedstock by source. LC-NFAX and HC-NFAX consider an additional input of 11 MtC (2–4%) from pyrolysed plastics, which was neglected by us.



infrastructure is still in its infancy and that geological storage capacities are limiting.⁴⁶

A rough calculation of the total carbon feedstock volumes based on their approximate carbon content (natural gas 75% C, dry wood 50% C,⁴⁷ CO₂ 27% C) indicates that the total feedstock amounts also differed considerably ranging from at least 688 Mt in modesty scenario HC-NFAX to an enormous amount of 6227 Mt in NZE2050H assuming the highest chemical demand (see Fig. S3†). These results indicate that the infrastructural burden for feedstock supply will also differ considerably. Scaling of CCU and biomass utilisation requires the largest capacity increases due to the low-carbon content of the starting materials.

2.4. Energy requirement in net-zero transition scenarios

In addition to carbon feedstock, net-zero chemical industry requires energy for the reduction of feedstock and as process energy. If fossil fuels are used, most of this energy comes with the feedstock. However, as biomass is only partially redox reduced, and CO₂ is highly oxidised, surplus energy is required for the manufacturing of primary chemicals from these two carbon sources. Most of this energy is supplied in the form of hydrogen produced from water using renewable electricity. The energy input requirements across the net-zero transition scenarios are discussed in the subsequent sections.

ZERO1.5 requires the input of 25.8 PWh energy (Fig. 5A and B) with 28% originating from fossil fuels, 25% from biomass and 27% from the chemical energy of hydrogen. Electricity

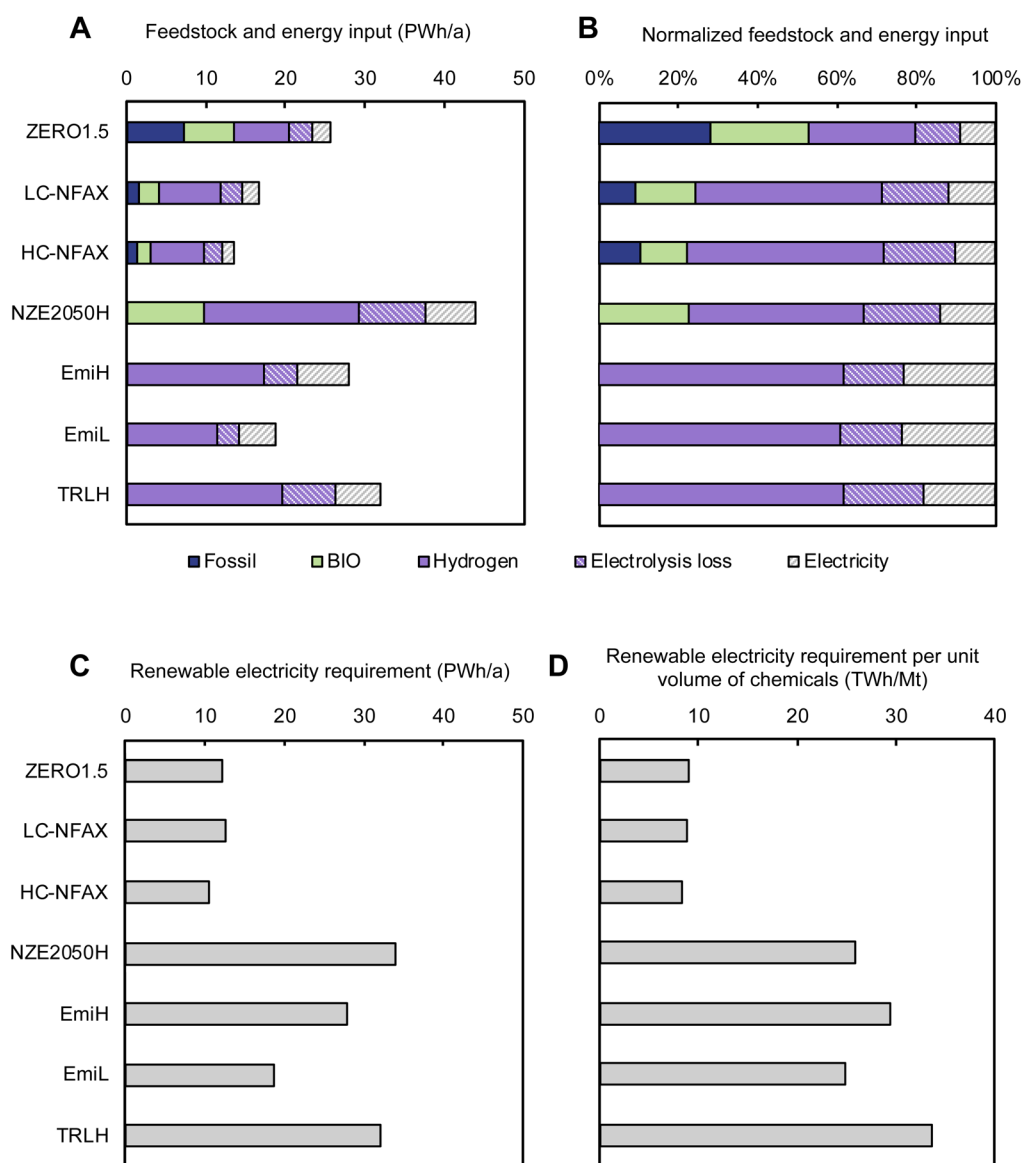


Fig. 5 Energy requirements for the analysed net-zero transition scenarios. Chemical energy and physical energy input as (A) totals or (B) normalised. Renewable electricity requirement, including electricity for hydrogen generation (chemical energy in hydrogen and losses occurring during electrolysis*) and electricity for manufacturing process, as (C) totals or (D) per unit volume of *de novo* synthesised chemicals. *The efficiency of electrolysis for hydrogen generation in the scenarios from top to bottom are 70%, 74%, 74%, 70%, 80%, 80% and 75%.

synthesised chemicals across the net-zero scenarios (Fig. 5D) is further evaluated. In scenarios where fossil fuels are not fully abated (ZERO1.5, LC-NFAX, and HC-NFAX), the extended use of these energy-dense feedstock can replace considerable fractions of renewable power. Hence, the electricity required per unit of chemicals in these scenarios is lower, ranging from 8.3 to 9.0 TWh per Mt.

In contrast, fully CCU-based net-zero transition scenarios (EmiH/EmiL and TRLH) are more energy intensive, leading to renewable electricity requirements per unit of chemicals of 24.9 to 33.7 TWh per Mt.

Biomass serves as a joker in the feedstock structure.⁵⁴ In NZE2050H, where 22% of the input energy is sourced from biomass, the renewable electricity requirement per unit of chemicals is 25.9 TWh per Mt. Biomass is more energy efficient compared to CCU and blending it into the carbon feedstock helps moderate the extremely high demand for electricity associated with CCU processes.

Compared with fossil inputs, with decreasing chemical energy content of starting materials (biomass and CO₂), renewable energy capacities must increase, with CCU being the most energy-intensive solution.^{55,56}

No single solution can shape the future of the chemical industry. To guide resource allocation and continuously enhance the system, a comprehensive evaluation including circularity, feedstock availability, and energy demand is necessary. Beyond the scientific disciplines, incorporating industry perspectives to evaluate its sustainability is also a powerful aid for decision-making.

3. Sustainability evaluation of defossilisation technologies

It is widely accepted to rest sustainability on a social, economic and environmental pillar⁵⁷ (Table 2). Here we want to evaluate different technological options for the manufacturing of primary chemicals and plastics (FOS, FOS/CCS, BIO, CCU) with regard to these three pillars of sustainability in order to assess their long-term perspective and to paint a bigger picture of defossilisation. The three-pillar concept was preferred by us as it is simpler than other proposed subdivisions, very well established in the public domain, and still allows for a sufficiently detailed analysis.

The rating we carried out takes into consideration the outcome of the technology's use "in a longer term". We considered the period up to 2050 to be appropriate primarily because it extends sufficiently far into the future, yet is nevertheless linked to specific political goals in important countries and regions^{58,59} such as Canada, China, the European Union, Japan, South Korea, the United Kingdom, and the United States, which stipulated binding goals to achieve climate neutrality around this year. In this way, we abstract from present-day issues, particularly the limited availability of renewable energy and a regulatory situation in need of development and can expect that key technologies in this area will have reached maturity. Also, the rating does not claim for itself to be

The standardised electricity input including hydrogen generation and process electricity of manufacturing *de novo*

Table 2 Rating criteria related to the three pillars of sustainability and their definition as applied in our rating

Environmental pillar	
Climate action	Refers to reducing greenhouse gas emissions
Biodiversity conservation	Refers to sustainable management of ecosystems, species, and genetic variability to maintain the delicate balance of life on Earth
Pollution prevention	Encompasses strategies and practices aimed at minimising or eliminating the creation of waste and pollutants to protect the environment and human health
Conservation of resources	Refers to the responsible and efficient use of natural resources to ensure their availability for present and future generations
Social pillar	
Health and well-being of the workers	Focuses on the physical, mental, and emotional health of workers, as well as access to healthcare services and support systems
Social equity and justice	This involves ensuring fair access to resources, opportunities, and benefits for all members of society, regardless of their background or circumstances
Community engagement and empowerment	Encouraging active participation, inclusivity, and empowerment of individuals and communities in decision-making processes that affect them
Economic pillar	
Job creation	Refers to the extent to which this technological option contributes to the creation of long-term and well-paid employment
Long-term success of sector-specific investments	Refers to the ability of an investment to generate positive returns and achieve its intended financial goals over an extended period of time. It takes into consideration factors such as the investment's performance, stability, and ability to withstand market fluctuations and economic cycles
Diversity (redundancy) of supply	Refers to the concept of having multiple sources or options for obtaining a particular product or service. It involves reducing reliance on a single source or supplier by diversifying and ensuring alternative sources are available. This approach helps mitigate risks associated with potential disruptions in the supply chain and enhances resilience in case of unforeseen events or challenges
Promoting technological innovation	Refers to activities, strategies, or initiatives aimed at fostering and encouraging the sustainable development and adoption of new advantageous technologies. It involves creating an environment that supports and incentivises the generation of novel ideas, research, and societal advancements in various fields

mathematically exact; rather, the year 2050 is used as an approximate reference point, which is essentially characterised by a state of affairs at which a number of advanced countries and regions should have achieved their long-term goals that they have set for themselves at present.

We have tried to choose the analysed focal points within the three pillars neutrally but are of course aware that other metrics or categories would yield different results. Of course, we are also aware that the identified components in a complex social system are interconnected and influence each other, unlike the basic variables in physical systems. The major intent was here again to highlight certain subaspects to get a sufficiently fair discussion without getting bogged down in the presently still existing uncertainties. We have therefore refrained from weighting the components. In a situation where the regulatory, fiscal and psychosocial conditions vary greatly (*e.g.* from country to country and region to region) and then change rapidly and individual economic area are facing pressure that urges them to reprioritise and divert from the ideal, weighting can become an empty academic exercise and outdated literally within months.

The rating presented here anyway does not claim mathematical precision but is rather a way of representation we have chosen to present a very diverse, complex context that is not easy to assess and in a state of flux. Our main aim was to provide an overall view of the environmental, economic, and social dimensions and drivers. Our rating is hence more of an instrument to structure our discussion and to motivate and

convey our point of view in a concise way. In quite a number of criteria, we assigned not just one rating value but a range to represent the variety of outcomes depending on factors, which are not inherent to the technologies but influenced by the specific conditions such as geographic location, social situation and the specific technical implementation. The researcher, technologist, economist, investor, citizen, or political decision-maker should be familiarised with the complexity but should not be lulled into a false sense of security that a specific technological solution provides with certainty a specific positive or negative outcome.

When analysing the results per pillar (see Tables 3 and S4–S14†), it is not entirely surprising that the technological options differ most clearly in the environmental pillar. For the environmental pillar, FOS is the worst, FOS/CSS is better and CCU best. BIO cannot simply be placed in a specific position in this string. BIO has the potential to contain very good but also rather unfavourable solutions which are hardly better than FOS in view of the environmental impact. The further BIO will develop from the first generation (biomass is derived from edible crops) through the second (non-food lignocellulosic biomass, including agricultural and forestry waste) to the third generation (algae and other microorganisms), the more positive its environmental profile will become. The third generation of BIO actually is essentially analogous to CCU only that the catalytic redox reduction is performed by biocatalysts instead of chemical catalysts and that the renewable energy for redox reduction comes from the sun, rather than from diverse sources like wind,



Table 3 Ratings for the sustainability of defossilisation technologies are based on environmental, social, and economic factors. See S4–S14 for detailed rubric

Rating criterion	Rating			
	FOS	FOS/CCS	BIO	CCU
Environmental pillar				
Climate action	—	0	−/0	0
Biodiversity conservation	—	—	−/0/+	+
Pollution prevention	—	—	−/0	0
Conservation of resources	—	—	−/0/+	+
Subtotal for environmental pillar	−4	−3	[−4, 2]	2
Social pillar				
Health and well-being	−/0/+	−/0/+	−/0/+	0/+
Social equity and justice	−/0/+	−/0/+	−/0/+	−/0/+
Community engagement and empowerment	−/0/+	−/0/+	−/0/+	−/0/+
Subtotal for social pillar	[−3, 3]	[−3, 3]	[−3, 3]	[−2, 3]
Economic pillar				
Job creation	−/0	0/+	0/+	+
Long-term success of an investment	—	0	−/0/+	−/0/+
Diversity (redundancy) of supply	—	—	0/+	0/+
Promoting technological innovation	−/0	0/+	−/0/+	+
Subtotal for economic pillar	[−4, −2]	[−1, 1]	[−2, 4]	[1, 4]
Total for all three pillars	[−11, −3]	[−7, 1]	[−9, 9]	[1, 9]

hydro, or solar. Furthermore: when it comes to the use of biogenic carbon dioxide through carbon capture and utilisation, the BIO and CCU scenarios can only be distinguished from one another by abstract definitions. For the sake of simplicity, we have refrained from rating the various forms of BIO separately in this assessment and have left it to emphasise the wide range of existing solutions and their very different levels of environmental sustainability.

In the social pillar, the four technological options do not vary *per se* from each other. They can be implemented in a socially responsible or antisocial way. These technological options are socially agnostic, so to speak. For the speed of technological transformation, it is of utmost importance that job cuts in extraction and processing of fossil carbon carriers are carried out in a socially acceptable manner and that affected regions are supported in the development of decarbonised and defossilised industries. Social problems in the affected regions promote the development of political forces that are hostile to and hinder the necessary technological change. There are numerous opportunities for socially acceptable change, which could include, for example, switching to the production of blue or turquoise or even green hydrogen.

Concerning the economic pillar, we see that there are intrinsically significant differences. However, the extent to which these differences will ultimately materialise and how quickly they will develop depends on political decisions and the legal framework that develops as a result.

The outcome of our rating is presented in Fig. 6. In all, we see a wide range of the outcomes of the ratings, which is a manifestation of the fact that much in the specific implementation can be done in a more or less sustainable way. FOS is in general the worst of all options, and even if in all free parameters, it is

implemented the best possible way, it will in the long run probably still be worse than the worst performance of CCU. We see the greatest spread of possible rating outcomes with BIO as

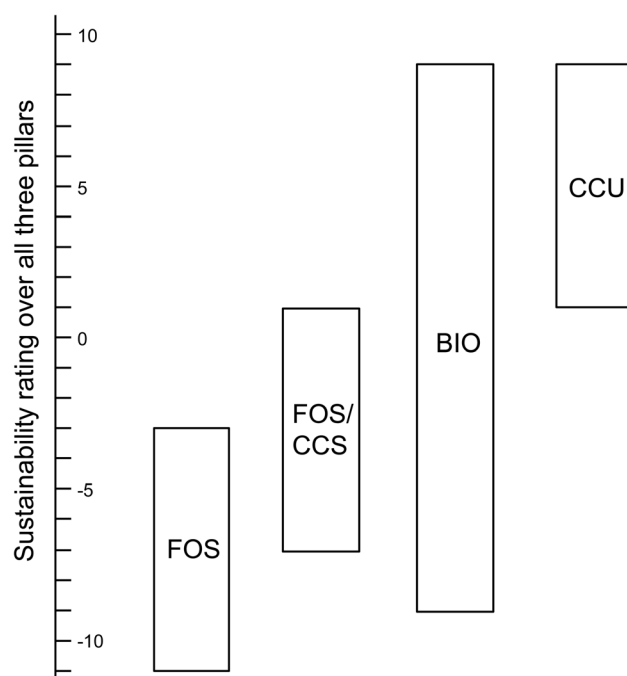


Fig. 6 Sustainability rating over environmental, social and economic pillars. The higher the position on the vertical scale the more sustainable a technological option performs. The length of the bar represents how different the sustainability of a technological option can be depending on the specific implementation. The rating is based on a long-term view which we define as the perspective until 2050.



was already discussed above. In its worst implementation, it is hardly better than FOS, while it can be as good as CCU in its best execution. Although FOS/CCS widely overlaps with FOS, it is in its best version for sure better than FOS but hardly reaches into the positive regions of well-implemented BIO and CCU. The broad ranges reflect our industry experience in the current pioneer era of defossilisation, where still only a small (but growing) number of product offerings are available. Each of these commercial solutions requires (besides the applicability assessment) a careful life-cycle assessment (LCA) of whether the non-fossil (presently mostly bio-based) product offered currently has a higher sustainability than as its fossil counterpart and how the profile may change in close future due to upcoming regulations (e.g. The EU's Carbon Border Adjustment Mechanism (CBAM)⁶⁰) or technological advancements.⁶¹

On the basis of the analysis presented here, we would like to take the liberty of making recommendations as to how, in our view, a successful and sustainable defossilisation of chemical industry, including plastics production, can best be promoted. Currently, in Europe, the use of sustainably generated electricity is being directed through legislative means to uses other than sustainable chemistry and particularly CCU, such as electromobility and modern heating technologies, especially heat pumps. This well make sense in the current situation, which is characterised by a lack of inexpensive, sustainably generated electricity, but in our view the legislature should step up promoting the expansion of sustainable electricity generation much more rigorously than it is presently done and, above all, should keep firmly in mind that the need to defossilise chemical industry, including plastics production, will require considerable capacities in the coming years.

Moreover, in our view, the potential synergies between CCS and CCU still receive too little attention from political decision-makers in Europe. The infrastructure to be created in the area of carbon capture and sequestration (carbon capture installations and pipeline networks) can be directly linked to that of carbon utilisation (CCUS). Further, if, for example, as in Switzerland,⁶² the CO₂ from waste incineration plants, which contains a substantial portion of CO₂ of biogenic origin (from food waste, soiled cardboard and paper, etc.), is captured, this carbon stream can partly be equated, in the sense of a mass balance approach, to that of bioenergy with carbon capture and storage (BECCS).^{63,64}

We thus find ourselves in an environment with risks and opportunities that invites us to actively and consciously shape the future of tomorrow's chemical industry with courage and confidence. The complexity identified should not deter the scientific-technical, economic, or political players from resolutely defossilising chemical industry, but rather encourage them to find the best possible solutions, which will undoubtedly not be without compromise. For a positive development, it would be important to convince larger sections of society of the benefits of technological development and to inspire enthusiasm for technological progress. As we saw, the technological options do not *per se* have social advantages over each other. This makes it all the more important that environmentally friendly technologies are well explained and then implemented

in such a way that local people experience social-economic progress when the technologies are introduced and therefore welcome and support them.

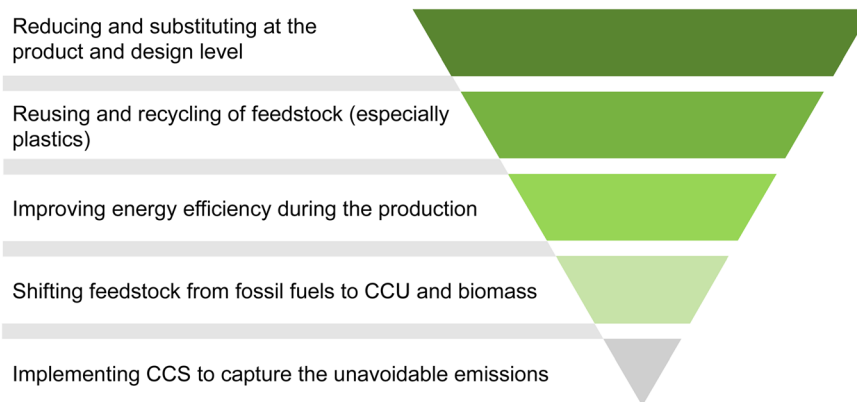
4. Discussion

Transitioning from a fossil-based to a net-zero chemical industry requires efforts from both the demand and supply sides. On the carbon supply side, there is agreement in all of the analysed net-zero transition scenarios that virgin fossil feedstock has to be decreased considerably, while non-fossil carbon from biomass or CO₂ needs to be ramped up to provide at least 60% of the carbon skeleton for *de novo* synthesised chemicals. On the demand side, shifting consumer habits and intensified recycling are key to curbing demand for *de novo* synthesised chemicals (especially the high-energy and carbon-loaded HVCs predominately used for plastic production) and thus ease energy and feedstock need. This shift is accompanied by a considerably growing future demand for chemicals in general and an eventually growing market for ammonia and methanol as energy carriers. As both the feedstock supply and the chemical demand side will change considerably, the material flow of the chemical industry will have to be rewired. The subsequent transition will undoubtedly pose a challenge to scientific research and technological development, investors, manufacturers, and consumers but also to the energy sector. However, as feedstock supply from biomass or captured atmospheric carbon is still underdeveloped, an important task for policymakers is to set up a framework that governs their exploitation.

4.1. Demand-side solutions: changing purchasing policies of industrial downstream users

From the consumer perspective, more and more companies including large multinationals, have been working on or even actively implementing purchasing guidelines aimed at requesting and evaluating non-fossil alternatives to their existing purchased product and raw material portfolio. The easiest way for the downstream user to replace the product is, of course, if substitute materials come with an LCA indicating superior eco-performance but are otherwise identical to the conventional product. The biggest challenge in this simplest of cases is to ensure that no regrettable substitution is allowed and/or that the price of the non-fossil alternative makes the resulting product so expensive that it is no longer competitive. Regrettable substitutions can only be avoided by thoroughly conducting LCA, also prospecting the impact of future improvements (e.g. an increasing share of energy from renewable sources), and carefully and critically reviewing the LCA data of the currently used materials.^{61,65,66} As far as potentially higher prices are concerned, it is hoped that the manufacturers of high-value and/or prestigious products with a small cost contribution of the raw materials to the sales price⁶⁷ will also want to play a pioneering role in line with their good reputation and particular sustainability ambitions, until increasing production volumes will help to bring prices further down.





- Recycling and reducing per capita consumption especially in the HVCs sector are absolutely important in reducing both raw material and energy requirements.

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