Planet compatible pathways for transitioning the chemical industry

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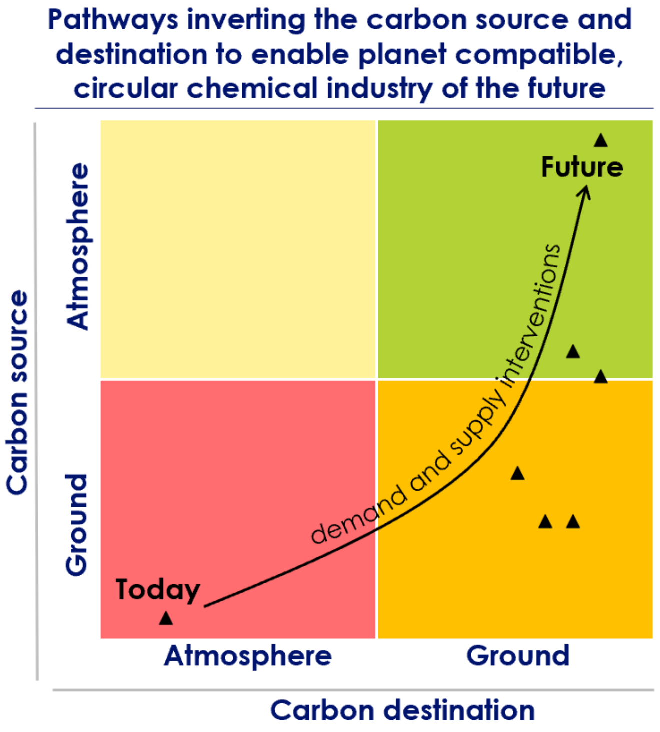
Abstract:

Chemical products, such as plastics, solvents, and fertilizers, are essential for supporting modern lifestyles. Yet, producing, using and disposing of chemicals creates adverse environmental impacts which threaten the industry's license to operate. This study presents seven planet compatible pathways towards 2050 employing demand-side and supply-side interventions with total investment costs of US$1.2-3.7 billion. Resource efficiency and circularity interventions reduce global chemicals demand by 23–33% and are critical for mitigating risks associated with using fossil feedstocks and carbon capture and sequestration, and constraints on available biogenic and recyclate feedstocks. Replacing fossil feedstocks with biogenic/air-capture sources, shifting carbon destinations from atmosphere to ground, and electrifying/decarbonizing energy supply for production technologies, could enable net negative emissions of 200 MtCO$_{2eq}$ yr^{-1}, while still delivering essential chemical-based services to society.

One-Sentence Summary:

Our study presents seven planet compatible pathways for transitioning the chemical industry towards net-zero, which rely on circular strategies and a new system service for sequestering carbon, while continuing to provide essential services to society.

TOC Figure:



Pathways inverting the carbon source and destination to enable planet compatible, circular chemical industry of the future

Introduction

The modern chemical industry stands at a crossroads. Following decades of fast-paced growth, chemicals and their derivatives are now ubiquitous in society (*1*, *2*) and essential for supporting modern lifestyles, contributing over 7% of global domestic product (GDP) in 2017 (*3*). Moreover, in the future, chemicals will likely play a significant role in delivering net-zero targets (e.g., ammonia for shipping). However, the industry faces multiple planet-wide environmental dilemmas. Energy-intensive chemical production processes consumed 14% of global oil and 9% of global gas, and released 13% of global industrial direct CO_2 emissions in 2020 (*4*, *5*). More greenhouse gases (GHGs) are released in upstream and downstream of production, including fugitive methane from upstream extraction processes(*6*–*9*), CO_2 from end-of-life plastics incineration (*10*), nitrous oxide (N_2O) from fertilizer application (*11*), and indirect GHGs from the generation of electricity and heat (*12*). Predominantly linear value chains, agricultural inputs and expanding land-use generate further environmental impact. For example, approximately 57% of the nitrogen in fertilizers is not absorbed by plants but instead finds its way into waterways and oceans (*13*–*15*), where it is joined by an estimated 11 Mt yr^{-1} of plastics leaked from ineffective waste management systems (*15*–*18*).

At the heart of these issues is the uncontrolled leakage of chemicals to the environment, via GHG emissions to the air and products to land, waterways and marine environments (*15*, *19*–*22*). This leakage has adverse effects on climate, biodiversity, ecosystems, and human health. Safeguarding planetary boundaries requires a transition towards more sustainable production and consumption of chemicals, where leakage is eliminated or made harmless to the environment and emissions are reduced across all lifecycle stages (*23*).

Yet, the road ahead for chemicals is divided. The industry’s preferred pathways to net-zero is to retrofit current chemical facilities with supply-based emissions mitigation solutions, while leaving demand for chemicals unconstrained. Supply-side technology options include carbon capture and storage (CCS) and utilisation (CCU), bio-based/green hydrogen-based feedstocks, direct air capture (DAC), and electrification. Given these technologies are yet to be deployed at meaningful scale (*25*), there is a significant risk of missing targets and locking in polluting systems by relying exclusively on this pathway. Opposing pathways, for instance, calls for bans on plastics (*26*) or a move to 100% material circularity (*27*). This pathway is equally risky, as there is often no better alternative to plastics, making bans impractical (*1*), and full material recovery is limited by thermodynamics laws, and thus unattainable (*28*) (e.g., for fertilizer dissipation in the environment).

Given the risks in pursuing these pathways, new options must be found between these extremes, that are feasible and able to mitigate planetary boundary risks to acceptable levels. This study aims to overcome the limitations of previously developed pathways (*1*, *25*, *27*, *29*), by exploring net-zero emissions pathways that employ both demand-side and supply-side mitigation strategies, while applying constraints on technology (e.g., CCS) and to feedstock availability (e.g., bio-based and recyclates) based on planetary boundaries. The result is lower-risk, technologically and financially feasible pathways which extend the solution frontier and place the chemical industry on a trajectory to meet 1.5°C, 2050 targets, while respecting planetary boundaries.

Methods

This study aims to identify and outline the key conditions for the chemical industry to reach net-zero GHG emissions along planet compatible pathways between 2020 and 2050. Emissions from feedstock sourcing, production, use phase and end-of-life emissions are considered (Table S1). We construct a dynamic production facility supply model, based almost exclusively on open-source data, which responds to different inputs (e.g., cost, carbon abatement, feedstock) and 50 production technologies (Figure S19), across 10 geographic regions. We focus on eight primary chemicals: ammonia, methanol, olefins (ethylene, propylene, butadiene), aromatics (benzene, toluene, xylene), and two derivatives (ammonium nitrate, urea) that currently account for ~72% of global chemical industry production GHG emissions, two-thirds of energy used, and ~82% of primary chemical production by mass.

Planetary boundaries and resource availability

The planetary boundaries framework identifies human perturbations in nine Earth system features that if transgressed will threaten the safe operating space for global societal development (*30*, *31*). This study selects climate change (GHG emissions) as a key modelling constraint, and considers available biomass (at 10 EJ or 720 Mt dry biomass for chemical use in 2050, ~20% of global availability) to safeguard land-system change and biodiversity (*32*). Impact on novel entities (e.g., plastic pollution into environment (*20*)) and biochemical flows (nitrogen) are assessed outside the main model.

For each chemical, we define planet compatible pathways to minimize demand for new chemical production and life cycle GHG emissions by 2050, with demand and supply strategies modelled concurrently. Resource efficiency and materials circularity (i.e., elimination, reuse, recycling, and substitution)[1] are presumed as key enablers for reducing demand for virgin chemicals and related emissions.

Demand scenarios

Business-as-usual demand (BDEM) scenario for chemical products is based on IEA RTS projections (*1*, *33*) plus additional demands for chemical products (ammonia for shipping and power generation; olefins for solar and wind deployment and electric mobility) required for net-zero pathways in other sectors (*34*, *35*).

Two demand scenarios are created based on BDEM with more ambitious shifts in end-use chemical demand: high circularity (HC) based on the maximum potential implementation of resource efficiency and circularity levers[2], low circularity (LC) at 50% of the maximum potential (except mechanical recycling using same absolute market size). Increases in resource efficiency and material circularity are considered for fertilizers, packaging, household goods,

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[1] The strategies of resource efficiency and circularity are defined inconsistently across literature. In this paper, we use both terms interchangeably, in their broadest sense, to cover solutions including elimination, reuse, recycling and substitution. Both resource efficiency and circularity strategies lead to reduce demand for virgin chemical production.

[2] There remain two large uncertainties associated with demand scenarios: (1) the baseline demand used from IEA may not be considered socially acceptable as the plastic and fertilizer consumption per capita in 2050 still includes large differences between countries and (2) the risk that, due to falling demand, oversupply from some production processes may remove local incentive for further demand reduction.

transportation, construction, and textiles, covering 87% of the chemical production studied here. For example, mechanical recycling is capped at optimistic 20-60% rates depending on plastics and sectors; see SI Section 4, Figure S2-12, Table S2-8.

HC and LC scenarios assume significant improvements in waste management (collection, sorting), end-of-life infrastructure (landfill, incinerators, CCS for incineration) and fertilizer application and use-efficiency. End-of-life emissions are calculated based on the demand scenarios (*15*).

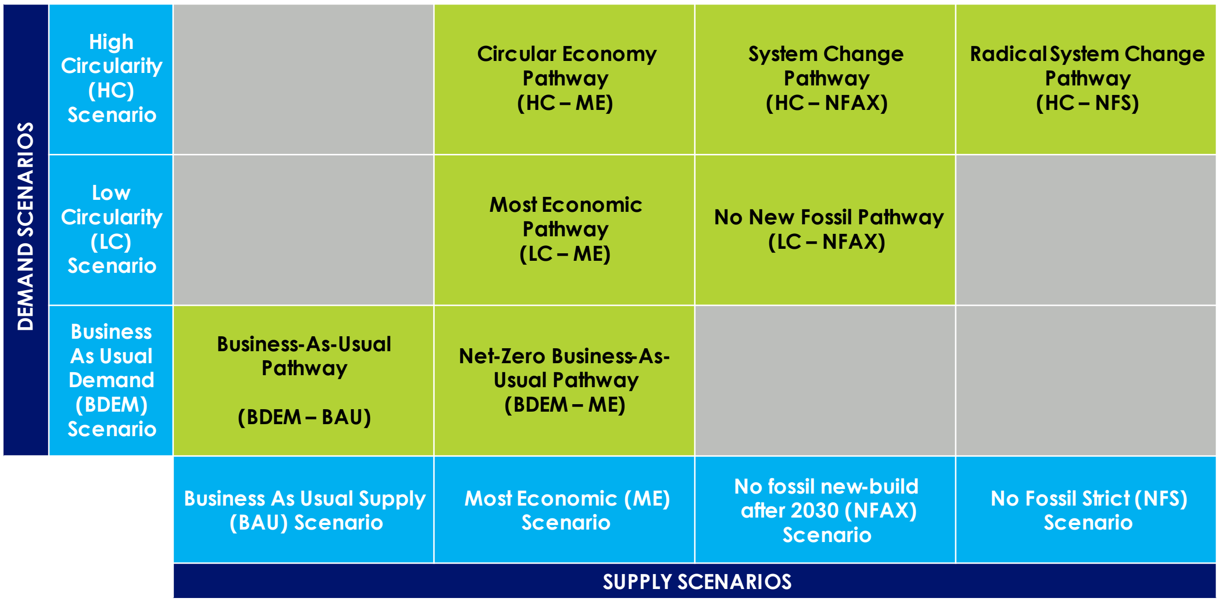
Supply scenarios

Only technically mature (>TRL 6) chemical production technologies are modelled to ensure pathways are technologically and financially realistic and immediately implementable. Evolving caps are applied to feedstocks and resources, including: sustainable biomass (*32*) (increasing from 2 to 12 EJ in 2050 including municipal solid waste; 25 % of share for chemical industry of global availability); polymer waste as feedstock for pyrolysis oil (~40 Mt yr^{-1}); treated wastewater (155 Gt yr^{-1}); and CO_2 storage (increasing from 0.04 to 1.75 Gt in 2050; 25% share for chemical industry of 7 Gt global CCS demand (*36*)). These limits are developed alongside projected demand in other sectors (e.g., aviation and steel) based on the IEA RTS scenarios and analysis by the Mission Possible Partnership. CCS is limited by a lack of current commercial scale storage facilities and CO_2 transport network, both of which have significant development timelines. In addition, localized geographical availability of underground CO_2 storage hinders wide-spread deployment, limiting build-out especially in the next 10–15 years (Fig. S26). Electrification, decarbonization of the power system and green hydrogen as a feedstock/storage medium underpin net-zero pathways for all sectors, and are not capped in the model due to shorter development timelines and no inherent physical or geographical limitations which could hamper roll-out (e.g., minerals, land availability) minerals, land availability).(*29*, *34–36*).

Four supply scenarios are developed: business-as-usual (BAU), most economic (ME), no fossil new-build after 2030 (NFAX) and no fossil strict (NFS). BAU selects the most economic technologies (including unabated), based on levelized cost of production, to meet demand, without considering emissions reduction. For all scenarios unabated fossil technologies can be built until 2025, beyond which only abated technologies (ME, NFAX, NFS) are allowed. NFAX builds no new fossil feedstock or energy plants after 2030 (even with CCS), while NFS, in addition, prevents any fossil-based feedstock or energy plant after 2025 and retires all fossil-based plants by 2050. An assumed fixed retrofit rate (5% yr^{-1} globally) is applied to convert or retire existing assets, with new plants optimized for lowest cost (ME) or largest GHG lifecycle emissions abatement (NFAX, NFS; see SI Section 5, Fig. S13-26).

Supply- and demand- pathways

This study features seven planet compatible pathways (shown in Table 1) selected as the most interesting pathways to compare and contrast. These pathways are not forecasts, but describe what needs to happen, based upon best available data today, to shift towards net-zero using different approaches. The pathways do not consider national infrastructure, trade, or energy security. Cumulative investment costs and levelized production costs (capital expenditures and operating expenses discounted to a present value per unit of production) are calculated using plant level modelling for each pathway, between 2020 and 2050.



DEMAND SCENARIOS	High Circularity (HC) Scenario		Circular Economy Pathway (HC – ME)	System Change Pathway (HC – NFAX)	Radical System Change Pathway (HC – NFS)
	Low Circularity (LC) Scenario		Most Economic Pathway (LC – ME)	No New Fossil Pathway (LC – NFAX)	
	Business As Usual Demand (BDEM) Scenario	Business-As-Usual Pathway (BDEM – BAU)	Net-Zero Business-As-Usual Pathway (BDEM – ME)		
		Business As Usual Supply (BAU) Scenario	Most Economic (ME) Scenario	No fossil new-build after 2030 (NFAX) Scenario	No Fossil Strict (NFS) Scenario
		SUPPLY SCENARIOS			

Table 1 The seven featured planet compatible pathways (green) combining demand and supply scenarios (blue). Detailed descriptions of each scenario can be found in Figure S14.

Results

Future projected demand for chemicals

Projected demand for the analysed chemicals increases rapidly between 2020 and 2050, assuming no toxicity regulatory changes of chemical uses (see SI Section 4). This is primarily driven by new demand for chemical products, which is partially offset by resource efficiency and circularity strategies (Figure 1). Demand excluding methanol demand for MTX rises from 693 Mt in 2020 to 1768 Mt in 2050 in the BAU scenario but is reduced to 1415 Mt (20% reduction) in the LC scenario and to 1261 Mt (29% reduction) in the HC scenario.

Today's ammonia production of 185 Mt represents 27% of the total chemicals produced, with ~70% used for nitrogen fertilizers. Ammonia for fertilizer use increases from 132 Mt (2020) to 158 Mt (2050) in the BAU scenario, while improved agricultural practices, diet shift and food waste reduction lower demand to 140 Mt (2050, LC) and 112 Mt (2050, HC) respectively. Ammonia is a promising pathway for decarbonizing long-distance marine transport and power in countries with highly limited renewables resources (*15*, *16*, *18*, *33*). New demand means ammonia production accounts for ~900 Mt of the total primary chemicals (~ 60%, BDEM) in 2050.

Today, methanol provides an alternative feedstock for diversified end-products: 28% for polymers (i.e., polyethylene and polypropylene via methanol-to-olefin (MTO) route), 22% for predominately resins (via formaldehyde derivatives), 27% for fuel, and the remainder for other chemical products. In the presented pathways, methanol emerges as a new carbon platform chemical, with 200-900 Mt being converted to olefins via methanol-to-olefins/propylene (MTO/P) and to aromatics via methanol-to-aromatics (MTA).

Three major olefins accounting for 290 Mt in 2020 (ethylene (56%), propylene (39%) and butadiene (5%)) are used in a wide range of products, dominated by polymers (~84%). Resource efficiency and circular strategies are leveraged by four downstream industries – transportation, construction, fast moving goods and textiles – reducing overall demand for olefins by 26–42% between 2020 and 2050. However, demand for ethylene in the energy sector increases by 27 Mt, driven by deployment of wind and solar technologies. Solar panels require specialty chemicals such as ethylvinylacetate or polyvinylfluoride, while wind turbine blades require polyethylene terephthalate for core structural components and chemicals for composite materials (e.g., epoxy, polyvinyl chloride, polyurethane) (*37*). Current demand for aromatics is 116 Mt, including benzene (36%), toluene (23%), xylenes (40%)), and is expected to remain flat until 2050 with downstream mechanical recycling providing an important feedstock.

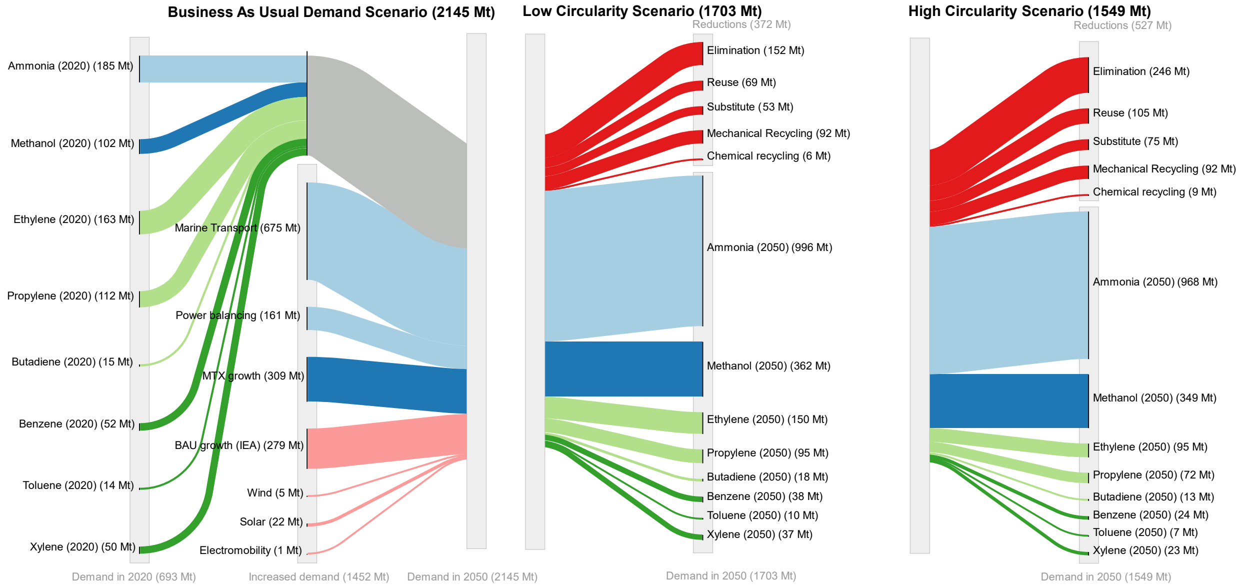


Figure 1 Material demand changes (in Mt) of eight primary chemicals (ammonium nitrate and urea shown as part of ammonia) between 2020 and 2050 under Low Circularity (LC), High Circularity (HC) and Business as Usual Demand (BDEM) scenarios, respectively. MTX growth is dependent on supply scenario and illustrated for LC-ME. Flow width indicates the masses of chemicals; flow color is used to distinguish different types of chemicals; grey indicates the BAU demand in 2020; red shows demand reduction through resource efficiency and circularity strategies, with improvements in agricultural practices included in the elimination wedge. Yearly volumes of each chemical over time including their supply technology mix can be found in Figures S27–S96. Chemical recycling in this study represents depolymerization and degradation (see SI Section 4.10).

Alternative feedstock, technology and process energy options

Reducing emissions from the chemical sector requires the combined use of alternative feedstocks, renewable energy for direct electrification and green hydrogen, CCS of CO_2 emissions (*38*), and efficiency improvements for heating processes to reduce the final energy demand.

Figure 2 illustrates key results across the presented pathways. Cumulative emissions account for 7–24% of the 1.5°C global carbon budget by 2050 (510 $GtCO_{2eq}$, 50% probability of limiting the global temperature below 1.5°C) (*21*). The most economic pathways (BDEM-ME, LC-ME, and

HC-ME) show the chemical industry using 8–9% of the 1.5°C global CO_2 budget available by 2050 (cumulative GHG emissions of 42–47 $GtCO_{2eq}$), the difference resulting from higher levels of resource efficiency and circularity, and more aggressive abatement. This requires 0.45–0.85 Gt CO_2 to be captured in 2050, equivalent to 25–50% of the CCS storage cap. In the early phase of the transition, this cap severely limits the deployment of CCS (Fig. S26). The LC/HC-NFAX and HC-NFS pathways produce only 36 $GtCO_{2eq}$ cumulative emissions (~ 7% of the global CO_2 budget), while lowering the demand for CCS to 0.16–0.31 $GtCO_{2eq}$/year.

Today's chemical system uses >99% fossil feedstocks, but by 2050 this declines to 42% (LC-ME) or more radically to <10 % (LC-NFAX and HC-NFAX) or 0% (HC-NFS), reducing cumulative emissions by about 20% (39–41 $GtCO_{2eq}$). Naphtha consumption drops most steeply (75-95% in LC-ME and LC-NFAX), due to the electrification of road transport and the consequent retirement of catalytic reforming, which produces approximately 85% of aromatics today. This is closely followed by coal (70-93% in LC-ME and LC-NFAX), which is disadvantaged in the model due to its higher emissions intensity and costs.

A large fraction (about 90%) of renewable energy used in the chemical industry in 2050 is for the production of green hydrogen, of which the large majority (>98%) is used as feedstock for ammonia and methanol production. Most methanol is converted to other products through MTO/P and MTA. We expect the chemical industry to remain the major producer and consumer of green hydrogen with up to 250 Mt needed in the no-fossil pathways, equal to 40–50% of global consumption in the 1.5°C aligned 2050 scenario (*29*, *35*). Approximately 250 Mt of sustainable biomass and municipal solid waste are needed in the no-fossil pathways, roughly equal to 40–50% of global consumption in the 1.5°C aligned pathway by 2050 (*29*, *35*), but play a minor role as feedstock and energy carriers (up to maximum 15% in HC-NFS).

CCU from point source emissions of CO_2 in industrial plants (e.g., steel, cement) plays a role in all pathways in methanol production. DAC provides a carbon source for the NFAX and NFS pathways and is favoured due to its negative emissions footprint and higher abatement potential. Specific technology makeups for each scenario are shown in Figures S27–S96.

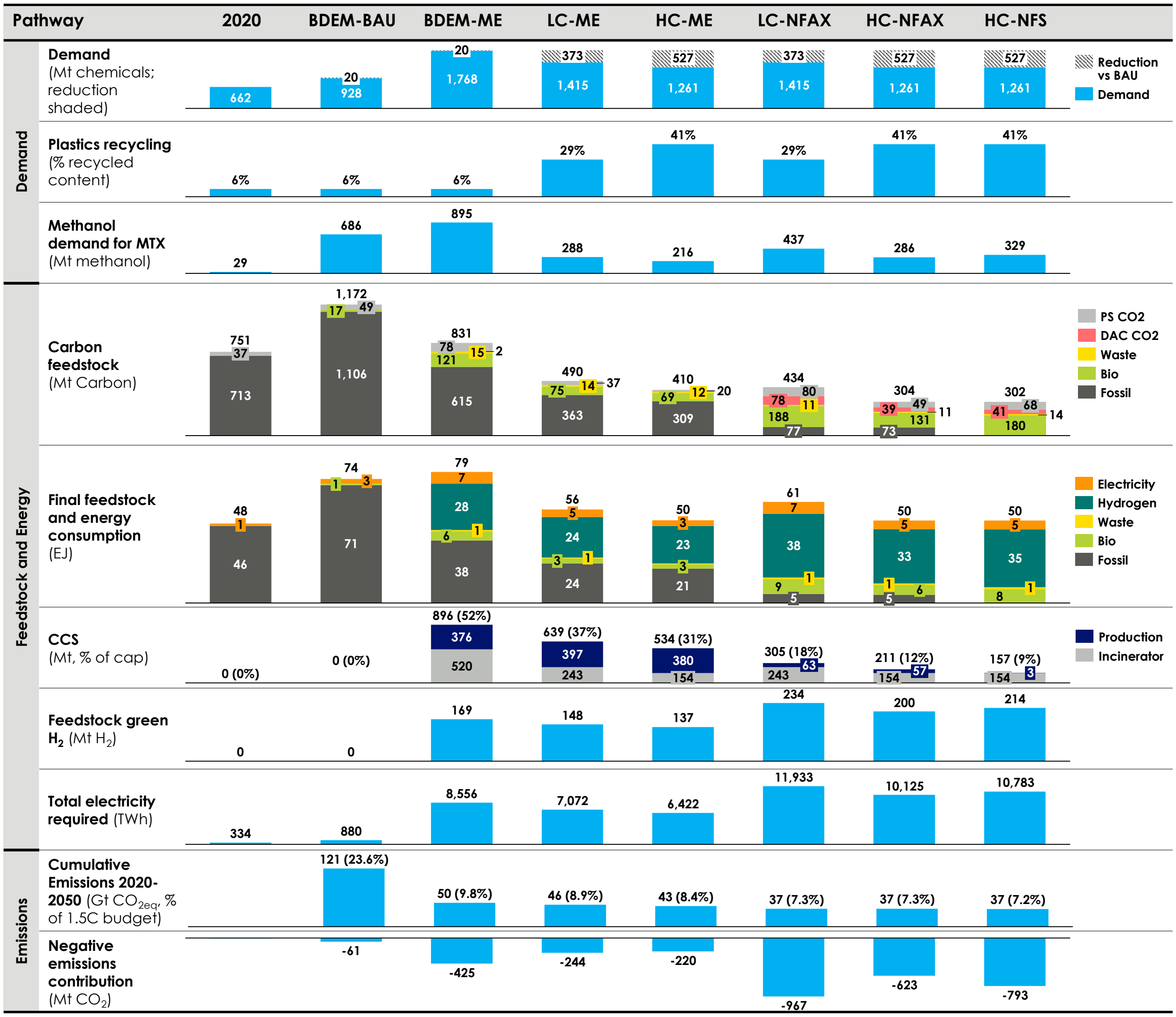


Figure 2 Emission mitigation strategies for all pathways. Demand in first row excludes methanol demand for MTX to avoid double counting. Reduction of demand in first row is shaded. Recycled content is different from recycling rates (see SI section 4.8 for definitions). Electricity for all scenarios besides BDEM-BAU is 100% renewable electricity. BDEM-BAU does not account for new demand associated with energy transition (e.g., ammonia for shipping).

Emissions and the opportunity of carbon vector inversion

Figure 3A shows the shares of GHG emissions across the lifecycle stages in 2050 (feedstock extraction, production, use and end-of-life) for the four main chemical groups (olefins, aromatics, ammonia, and methanol) and seven featured pathways, compared with 2020. The lifecycle emissions profiles vary significantly across the chemical groups: for example, the use-phase emissions from fertilizer use dominate for ammonia (>90% across all emission reduction pathways), while for olefins, feedstock and end-of-life emissions are most important.

In 2020, the total contributions to annual emissions are: 36% (0.8 $GtCO_{2eq}$ yr^{-1}) from the production phase; 21% (0.5 $GtCO_{2eq}$ yr^{-1}) from the feedstock phase; 42% (1.0 $GtCO_{2eq}$ yr^{-1}) from the use- and end-of-life phases. Fugitive methane emissions are potentially underestimated (*39*), with some recent studies estimating fugitive emissions to be 25–40% larger, presenting a significant climate risk if unmitigated. End-of-life emissions across the industry would increase by up to 70% (2.3 $GtCO_{2eq}$ in 2020) if all plastic waste was incinerated, either with or without energy recovery. In this study, it is assumed that by 2050 existing and new waste incineration is abated with CCU or CCS technology.

By 2050, the share of global GHG emissions attributed to chemicals has changed: emissions are abated by new supply technologies and now contribute only 15–24% of lifecycle emissions in the ME pathways (remaining residues due to CCS) and 0–2% in the NFAX/NFS pathways. Use-phase emissions of fertilizers cannot be abated fully and contribute the largest share of positive emissions in each pathway in 2050 (27–52%)[3]. However, the NFAX and NFS pathways have negative emissions contributions from biomass and DAC, enabling an overall net-negative emissions profile and compensating for the unabated fertilizer use-phase emissions. For example, olefins production today depends heavily on naphtha and ethane for steam cracking. A switch to bio-oils and bioethanol dehydration renders emissions for feedstock production negative for olefins production, up to 0.2 $GtCO_{2eq}$ removed every year.

Figure 3B shows the trajectories of annual emissions from 2020 to 2050 for all pathways. NFAX and NFS pathways move away from fossil feedstocks and shift end-of-life carbon from atmospheric emissions to sequestration, to achieve up to ~0.20 Gt of carbon sequestration per year by 2050. Other pathways, however, are not able to reach full net-zero, largely due to the unmitigated GHG emissions from the fertilizer use-phase.

Figure 3C shows a 2x2 matrix that illustrates the direction of carbon flow (the carbon vector) between the ground and air. Today's business as usual trajectory for the chemical industry (BDEM-BAU) results in carbon flowing from the ground (as fossil fuels) to the atmosphere (as CO_2 and fugitive methane), as shown in the red square. The most economic pathways (-ME), commonly discussed in the industry today, rely on technologies that return carbon back to the ground (CCS, landfill) to lower emissions intensity. However, the more ambitious pathways (-NFAX and -NFS) require an inversion of the carbon vector, taking carbon from the atmosphere (DAC, bio) and sequestering it in the ground (CCS, landfill) to go beyond net-zero towards carbon negativity.

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[3] Strategies for reducing use-phase fertilizer emissions include: precision agriculture, using nitrification and urease inhibitors and substituting urea, urea ammonium nitrate and ammonium bicarbonate, with ammonium nitrate.

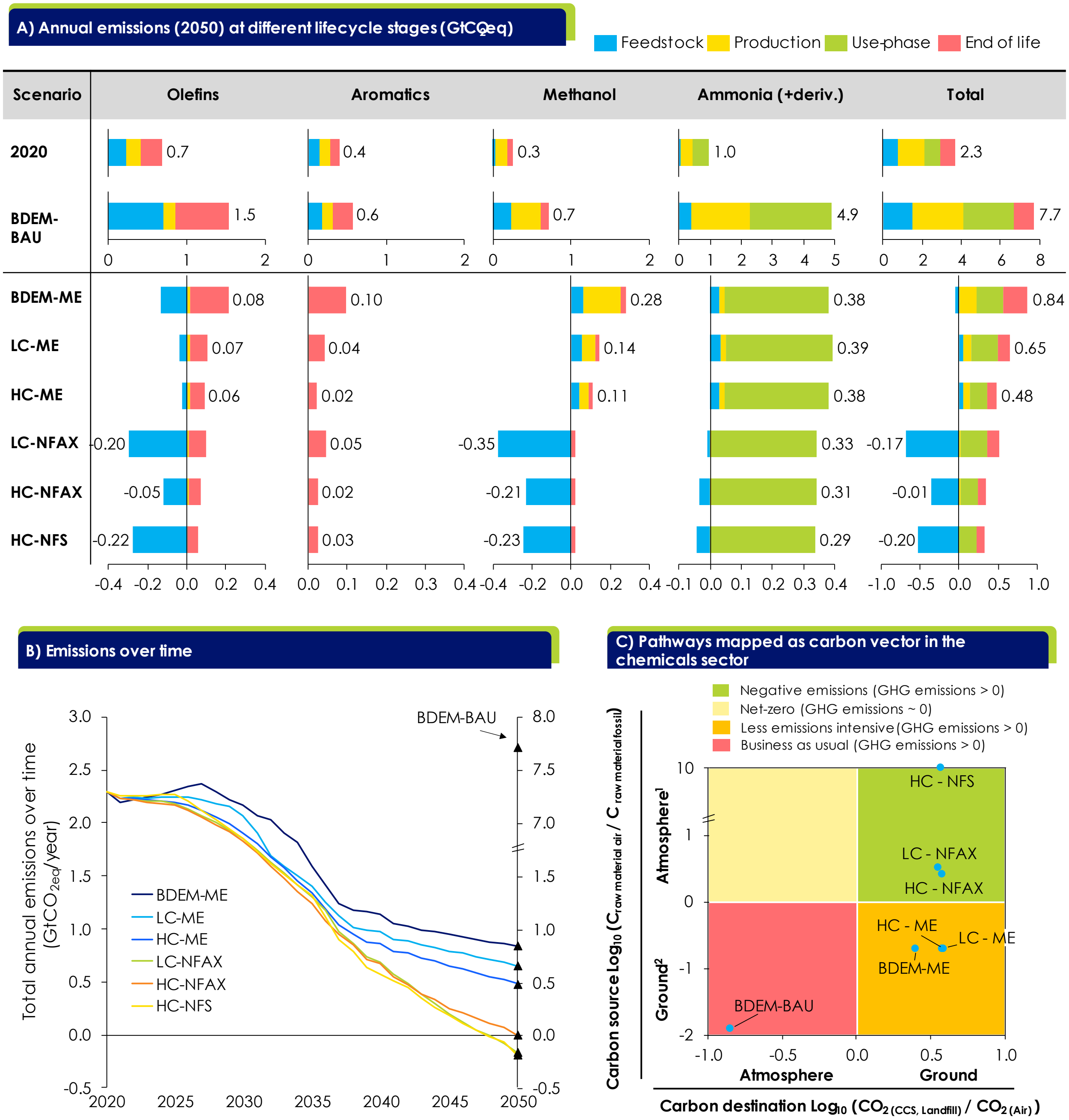


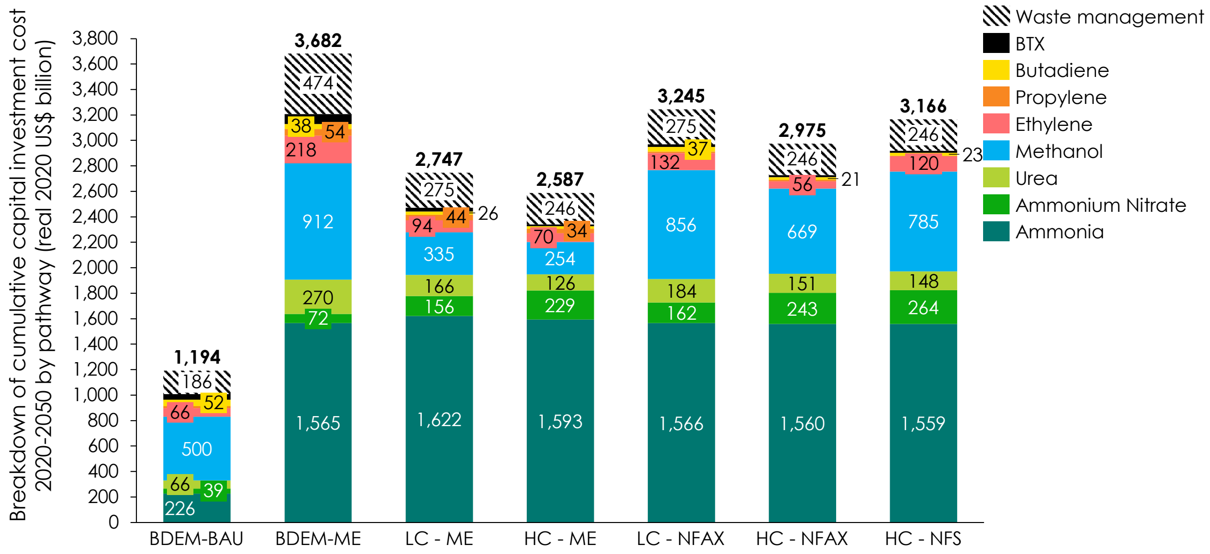
Figure 3 A) Annual GHG emissions of the analyzed chemicals in 2050 over the life cycles for all pathways considered in this study. Use-phase emissions are included for fertilizer but not for plastics; B) Total annual emissions from 2020 to 2050 including GHG emissions associated with fertilizer use-phase. Lower embodied carbon emissions in methanol used in MTA constructed in 2040s lead to diversion of the pathways after 2035. C) Carbon vectors between the ground (fossil) and atmosphere (biogenic or direct air captured carbon) with represented pathways. No pathway is in the top left box because of the assumption on 100% CCS of waste incineration.

Investment costs

The cumulative capital expenditure by 2050 to finance the LC-ME and LC-NFAX pathways is anticipated to be US$2.7 trillion and US$3.2 trillion, respectively, a 125–170% increase above BAU requirements (US$1.5–2.0 trillion). This includes investment costs for renewables for green hydrogen production as a feedstock, which contribute a large share (approximately 50–70%) of the total investment costs for green ammonia and methanol. In addition, $0.2–0.5 trillion is required in both pathways to manage production and end-of-life waste streams, including collection, sorting, recycling, landfill, incineration and associated CCS (Figure 4A).

Under the LC-NFAX pathway, the levelized production cost will almost double in 2050, compared to today. For example, the average cost of olefins will rise from $800–1000 to about $1400–2000 per metric ton (Figure 4B).

A) Investment cost



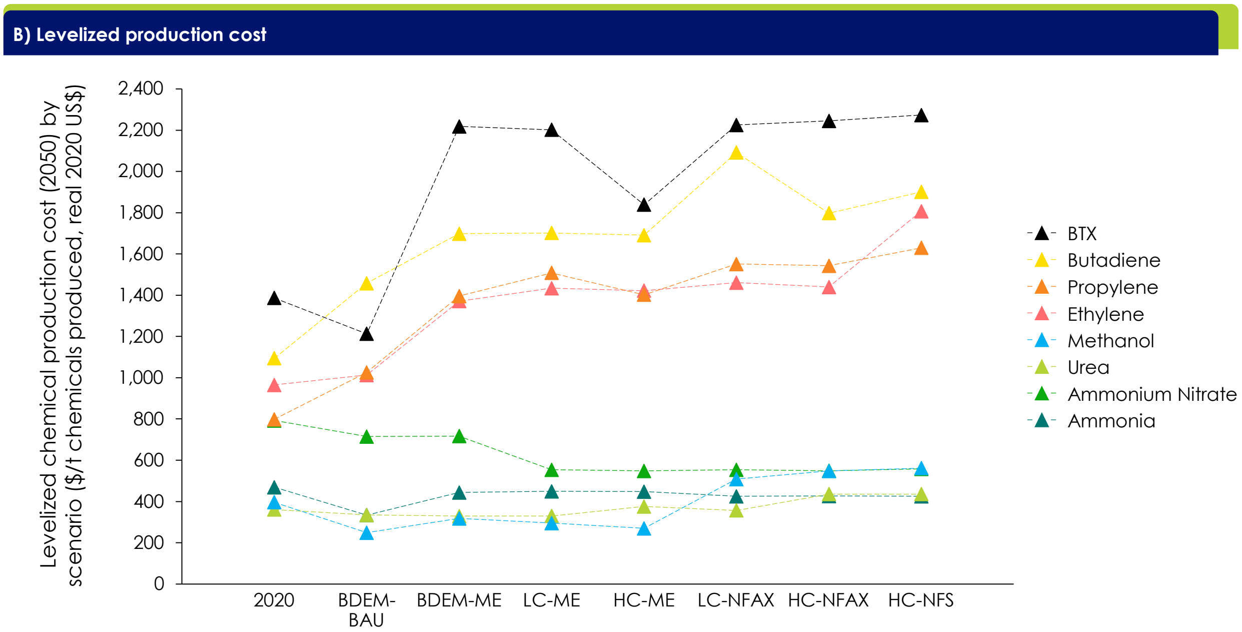


Figure 4 A) Breakdown of capital investment cost of all chemicals and pathways (US$ billion). B) Average levelized production costs of plant stack in 2050 (US$/t).

Discussion

This study explores a range of feasible, planet compatible net-zero emission pathways, which will allow the chemical industry to achieve 1.5°C targets by 2050. Our results show that reaching net-zero for the chemical sector requires supply-side emission abatement interventions that go beyond the most economical pathways (ME), towards low fossil feedstock pathways (NFAX and NFS). These interventions rely on a diverse set of supply technologies (e.g., DAC) and renewable feedstocks (e.g., biomass, green hydrogen), with high-risk. However, this risk is mitigated by reducing demand for virgin chemicals, through resource efficiency and circularity strategies, enabling the chemical industry to remain well within the tolerance of planetary boundaries and technology scaling limits.

Balancing carbon flows

Across all pathways, the key to delivering net-zero emissions lies in balancing carbon flows, a challenge which is unique to the chemical industry where carbon is embedded in products. Figure 5A compares embedded carbon in feedstocks (sourcing and production) and carbon destinations (end-of-life treatments) for chemical products. At each of the three levels, carbon flows need to be balanced to achieve net-zero emissions. First, the use of fossil-based feedstocks must be balanced with sequestration technologies (CCS of emissions or landfilling of products at end-of-life). CCS allocation to the chemicals industry is limited (assumed to be 470 Mt C or 1.75 $GtCO_{2eq}$ in 2050), placing a cap on the use of fossil-based feedstocks. Second, carbon in discarded chemical products can be recycled as a feedstock for new products. However, collection, sorting and recycling processes for plastics are imperfect, some plastics are challenging to recycle, and plastic material is degraded during recycling, limiting the available carbon from recyclates (~30 Mt C via pyrolysis, 74 Mt C via municipal waste gasification, 139 Mt C via reuse and recycling). Third, chemical products incinerated at end-of-life release carbon to the atmosphere, so must be discontinued or abated with carbon captured from the air, using bio-based feedstocks or DAC/CCU technologies. However, biomaterials are limited in supply (~350 Mt C) and DAC/CCU technologies are costly, energy- and resource- intensive.

The sum of these limits constrains available carbon for new chemical products (~1070 Mt C). However, considering practical, technical and economic requirements to utilize 100% of all these resources, suggest demand reduction to forecasted BAU demand (650 Mt C) to balance the carbon flows may be required. This sets up an explicit tradeoff between bio-based products, recycling, CCS and demand reduction. Under the assumptions in this study, a 23–33% demand reduction for chemical products from BAU facilitates a 9–12% reduction in cumulative emissions from 2020 to 2050 (LC-, HC-).

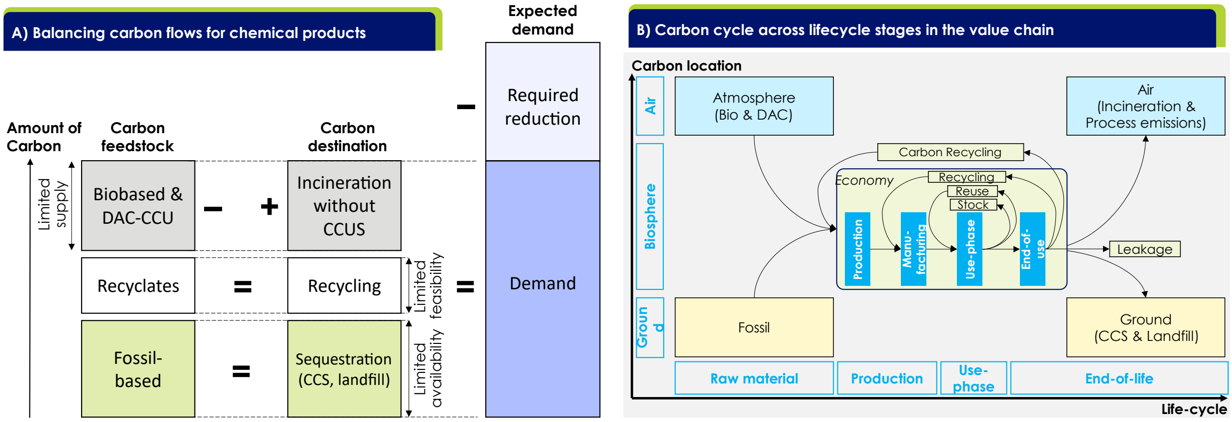


Figure 5 A) Net-zero and carbon balance require the carbon amount in corresponding boxes in feedstock and destination be the same, and together set a limit in the demand. Only CO_2 emissions related to embedded carbon are considered (i.e., carbons that go into chemical products of demand). Process emissions are outside the scope of the diagram and need to be dealt with separately by renewable energy, CCS, etc. B) Simplified carbon flows across lifecycle stages in the value chain.

Carbon vector change - from ground to air

The carbon balance also reveals a unique opportunity for the chemical industry to provide negative emissions, which may offset difficult to abate emissions in other sectors. Today's chemical processes mostly take carbon from the ground and release it to the atmosphere as emissions, creating a ground-to-air carbon vector (Figures 3C). However, the carbon cycle shows a possible route for inverting the carbon vector, to air-to-ground, by combining bio-based and DAC/CCU technologies with sequestration using CCS or landfill. This offers a new dual value proposition for the chemical industry: utility from chemical products and potentially an additional revenue stream from negative emissions. This unique path for the chemical industry adds significant value to society compared to e.g. DACCS without utilisation of the carbon atom.

However, relying solely on carbon sequestration technologies to mitigate emissions is risky, given their slow development and deployment to date (only ~40 Mt CCS capacity in 2020 (*31*)). To mitigate this risk, the industry should also pursue resource efficiency and material circularity solutions (in the centre of Figure 5B) to reduce overall demand for chemical products. Avoiding new virgin production solves several environmental impacts at once, mitigating emissions from extraction, production, and unabated incineration alongside leakage to waterways and marine environments.

Staying within the other planetary boundaries

Climate change is only one of the nine planetary boundaries processes, so the influence of our pathways' pursuit of net-zero on other processes is examined here. Land-system change is measured by the area (%) of forest land (*39*, *40*), and our pathways set a cap in the biomass availability such that no net conversion of forest takes place. Biochemical flow (nitrogen) is measured by industrial and biological fixation of nitrogen (*39*, *40*). If we assume that the use of ammonia as a fuel returns the fixated nitrogen back to molecular nitrogen, the net fixation of nitrogen in the LC (210 Mt yr^{-1} as ammonia) and HC (182 Mt yr^{-1}) demand pathways in 2050 is less than that in the BDEM pathways (228 Mt yr^{-1}). Persson et al. highlighted that novel entities, especially plastic pollution, are now considered to have exceeded the planetary boundary (*20*). Our demand pathways (-LC and –HC) release 22.1 Mt and 16.3 Mt per year of mismanaged plastic waste into oceans and land, respectively, less than BDEM pathways at 35.0 Mt yr^{-1}. We conclude that the pursuit of net-zero pathways outlined in this study is not at the expense of other planetary boundary processes and is beneficial, especially where demand reduction levers are deployed. The chemical industry could even have a positive impact on planetary boundaries through levers not studied here (e.g., reduced ecosystem exposure to toxic chemicals).

The impact on the cost of chemicals

The transformation of chemical industry will require changes to every single existing asset (decommissioning, retrofit, upgrade) to achieve net-zero. Resulting cost increases in basic chemicals, such as olefins and aromatics, will invariably impact the costs of end-user products, such as automotive and food products. This impact is estimated using an input-output price model and the Leontief inverse matrix for the United States in 2012 (*41*) and Japan in 2015 (*42*) (see SI Section 7). The analysis assumes that upstream price increases will be passed downstream and reflected in the price of purchased products without absorbing or inflating the price change, and without changing the production volume or input materials. A 100% cost increase (double the cost) of olefins and aromatics (but excluding ammonia and methanol) would cause the production cost of an automobile to increase by 1.1% and 1.0%, and (frozen) food products to increase by 0.9% and 0.6% in the US and Japan, respectively. Furthermore, the impact of doubling the cost of olefins and aromatics does not translate to the cost of end-user products, due to inputs and value added from all sectors in the supply chain (*43*). The implication is that the chemical industry should not delay the transition to net-zero, as any cost increase in primary chemicals will have an almost negligible impact on the production cost of end-user products.

Recommendations

This study has demonstrated that achieving net-zero emissions across the lifecycle stages for chemical products is possible but requires the deployment of both supply- and demand-side interventions. The chemical industry should accelerate the development of technologies highlighted in this study (non-fossil feedstocks as well as CCS, MTO/P and MTA), and collaborate across different industries to drive resource efficiency and material circularity, to reduce demand and balance the carbon flows. Policies such as carbon pricing and mandates to bridge the cost gap across the supply chain are essential to accelerate investment in the chemical industry. Additional revenue streams from negative emissions may offer a new value proposition for the industry. Demand-side coalitions and changes to government purchasing can help drive future demand for net-zero chemicals. In conclusion, this work highlights planet compatible pathways for the chemical industry based on circular strategies and a new system service for sequestering carbon, while continuing to provide essential services to society.

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Supplementary Materials

Materials and Methods

Supplementary Text

Figs. S1 to S97

Tables S1 to S12

References (*1*–53)

References

1. International Energy Agency, "The Future of Petrochemicals - Towards more sustainable plastics and fertilisers" (2018).

2. P. G. Levi, J. M. Cullen, Mapping Global Flows of Chemicals: From Fossil Fuel Feedstocks to Chemical Products. *Environ. Sci. Technol.* **52**, 1725–1734 (2018).

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

4. International Energy Agency, Tracking Industry 2021, (available at https://www.iea.org/reports/tracking-industry-2021).

5. International Energy Agency, Chemicals – Analysis, (available at https://www.iea.org/reports/chemicals).

6. D. T. Allen, A. P. Pacsi, D. W. Sullivan, D. Zavala-Araiza, M. Harrison, K. Keen, M. P. Fraser, A. Daniel Hill, R. F. Sawyer, J. H. Seinfeld, Methane Emissions from Process Equipment at Natural Gas Production Sites in the United States: Pneumatic Controllers. *Environ. Sci. Technol.* **49**, 633–640 (2015).

7. F. J. Cardoso-Saldaña, D. T. Allen, Projecting the Temporal Evolution of Methane Emissions from Oil and Gas Production Sites. *Environ. Sci. Technol.* **54**, 14172–14181 (2020).

8. R. A. Alvarez, D. Zavala-Araiza, D. R. Lyon, D. T. Allen, Z. R. Barkley, A. R. Brandt, K. J. Davis, S. C. Herndon, D. J. Jacob, A. Karion, E. A. Kort, B. K. Lamb, T. Lauvaux, J. D. Maasakkers, A. J. Marchese, M. Omara, S. W. Pacala, J. Peischl, A. L. Robinson, P. B. Shepson, C. Sweeney, A. Townsend-Small, S. C. Wofsy, S. P. Hamburg, Assessment of methane emissions from the U.S. oil and gas supply chain. *Science*. **361**, 186–188 (2018).

9. International Energy Agency, "Global Methane Tracker 2022 – Analysis," (available at https://www.iea.org/reports/global-methane-tracker-2022).

10. O. Eriksson, G. Finnveden, Plastic waste as a fuel **-** CO2-neutral or not? *Energy Environ. Sci.* **2**, 907–914 (2009).

11. X. Zhang, E. A. Davidson, D. L. Mauzerall, T. D. Searchinger, P. Dumas, Y. Shen, Managing nitrogen for sustainable development. *Nature*. **528**, 51–59 (2015).

12. International Energy Agency, IEA Sankey Diagram of World Final Consumption (2019), (available at https://www.iea.org/sankey/#?c=World&s=Final%20consumption).

13. U. N. E. Programme, *Marine Plastic Debris and Microplastics: Global Lessons and Research to Inspire Action and Guide Policy Change* (2016; https://wedocs.unep.org/xmlui/handle/20.500.11822/7720).

14. P. Paruta, M. Pucino, J. Boucher, "Plastic Paints the Environment" (2021), (available at https://www.e-a.earth/_files/ugd/425198_6f553fe5eb444350bb61b4acee3aef14.pdf).

15. W. W. Y. Lau, Y. Shiran, R. M. Bailey, E. Cook, M. R. Stuchtey, J. Koskella, C. A. Velis, L. Godfrey, J. Boucher, M. B. Murphy, R. C. Thompson, E. Jankowska, A. Castillo Castillo, T. D. Pilditch, B. Dixon, L. Koerselman, E. Kosior, E. Favoino, J. Gutberlet, S. Baulch, M. E. Atreya, D. Fischer, K. K. He, M. M. Petit, U. R. Sumaila, E. Neil, M. V. Bernhofen, K. Lawrence, J. E. Palardy, Evaluating scenarios toward zero plastic pollution. *Science*. **369**, 1455–1461 (2020).

16. R. Geyer, J. R. Jambeck, K. L. Law, Production, use, and fate of all plastics ever made. *Sci. Adv.* **3**, e1700782 (2017).

17. MacArthur, E., M. R. Stuchtey, K. Zumwinkel, "Growth Within: A circular economy vision for a competitive Europe" (Ellen MacArthur Foundation, 2015), (available at https://emf.thirdlight.com/link/8izw1qhml4ga-404tsz/@/preview/1?o).

18. OECD, *Improving Markets for Recycled Plastics: Trends, Prospects and Policy Responses* (OECD, 2018; https://www.oecd-ilibrary.org/environment/improving-markets-for-recycled-plastics_9789264301016-en).

19. Fertilizers Europe, "Carbon footprint reference values. Energy efficiency and greenhouse gas emissions in European mineral fertilizer production and use." (2011), (available at https://www.fertilizerseurope.com/wp-content/uploads/2020/01/The-carbon-footprint-of-fertilizer-production_Regional-reference-values.pdf).

20. L. Persson, B. M. Carney Almroth, C. D. Collins, S. Cornell, C. A. de Wit, M. L. Diamond, P. Fantke, M. Hassellöv, M. MacLeod, M. W. Ryberg, P. Søgaard Jørgensen, P. Villarrubia-Gómez, Z. Wang, M. Z. Hauschild, Outside the Safe Operating Space of the Planetary Boundary for Novel Entities. *Environ. Sci. Technol.* **56**, 1510–1521 (2022).

21. Intergovernmental Panel on Climate Change (IPCC), "Climate Change 2022 **-** Mitigation of Climate Change (Working Group III contribution to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change)" (2022), (available at https://report.ipcc.ch/ar6wg3/pdf/IPCC_AR6_WGIII_FinalDraft_FullReport.pdf).

22. U. N. Environment Programme, Global Chemicals Outlook. *UNEP - UN Environ. Programme* (2019), (available at http://www.unep.org/explore-topics/chemicals-waste/what-we-do/policy-and-governance/global-chemicals-outlook).

23. Naoko Ishi, Ani Dasgupta, Guillaume Lafortune, Jeremy Oppenheim, Johan Rockström, Guido Schmidt-Traub, Felix Cornehl, Astrid von Preussen, "Safeguarding the Global Commons for human prosperity and environmental sustainability" (2022), (available at https://cgc.ifi.u-tokyo.ac.jp/wp-content/uploads/2022/05/Safeguarding-the-Global-Commons.pdf).

24. A. Kätelhön, R. Meys, S. Deutz, S. Suh, A. Bardow, Climate change mitigation potential of carbon capture and utilization in the chemical industry. *Proc. Natl. Acad. Sci.* **116**, 11187–11194 (2019).

25. D. Saygin, D. Gielen, Zero-Emission Pathway for the Global Chemical and Petrochemical Sector. *Energies*, 28 (2021).

26. Á. Galán-Martín, V. Tulus, I. Díaz, C. Pozo, J. Pérez-Ramírez, G. Guillén-Gosálbez, Sustainability footprints of a renewable carbon transition for the petrochemical sector within planetary boundaries. *One Earth*. **4**, 565–583 (2021).

27. R. Meys, A. Kätelhön, M. Bachmann, B. Winter, C. Zibunas, S. Suh, A. Bardow, Achieving net-zero greenhouse gas emission plastics by a circular carbon economy. *Science*. **374**, 71–76 (2021).

28. J. M. Cullen, Circular Economy: Theoretical Benchmark or Perpetual Motion Machine? *J. Ind. Ecol.* **21**, 483–486 (2017).

29. International Energy Agency, "Net Zero by 2050" (2021), (available at https://www.iea.org/reports/net-zero-by-2050).

30. European Commission, "Landfill waste," (available at https://ec.europa.eu/environment/topics/waste-and-recycling/landfill-waste_en).

31. Global CCS Institute, "Global Status of CCS 2021: CCS accelerating to net zero" (2021), (available at https://www.globalccsinstitute.com/wp-content/uploads/2021/11/Global-Status-of-CCS-2021-Global-CCS-Institute-1121.pdf).

32. Energy Transition Commission, "Bioresources within a Net-Zero Emissions Economy: Making a Sustainable Approach Possible" (2021), (available at https://www.energy-transitions.org/publications/bioresources-within-a-net-zero-emissions-economy/).

33. International Energy Agency, *Ammonia Technology Roadmap: Towards more sustainable nitrogen fertiliser production* (OECD, 2021; https://www.oecd-ilibrary.org/energy/ammonia-technology-roadmap_f6daa4a0-en).

34. Energy Transition Commission, "Making Clean Electrification Possible: 30 Years to Electrify the Global Economy" (2021), (available at https://www.energy-transitions.org/wp-content/uploads/2021/04/ETC-Global-Power-Report-.pdf).

35. Energy Transitions Commission (ETC), "Making the Hydrogen Economy Possible: Accelerating Clean Hydrogen in an Electrified Economy" (2021), (available at https://energy-transitions.org/wp-content/uploads/2021/04/ETC-Global-Hydrogen-Report.pdf).

36. Energy Transitions Commission, "Carbon capture, utilisation and storage in the Energy Transition: Vital but limited" (2022).

37. European Commission. Joint Research Centre., “Raw materials demand for wind and solar PV technologies in the transition towards a decarbonised energy system.” (Publications Office, LU, 2020), (available at https://data.europa.eu/doi/10.2760/160859).

38. DECHEMA, “Low carbon energy and feedstock for the European chemical industry” (2017), (available at https://dechema.de/dechema_media/Downloads/Positionspapiere/Technology_study_Low_carbon_energy_and_feedstock_for_the_European_chemical_industry.pdf).

39. B. Hmiel, V. V. Petrenko, M. N. Dyonisius, C. Buizert, A. M. Smith, P. F. Place, C. Harth, R. Beaudette, Q. Hua, B. Yang, I. Vimont, S. E. Michel, J. P. Severinghaus, D. Etheridge, T. Bromley, J. Schmitt, X. Faïn, R. F. Weiss, E. Dlugokencky, Preindustrial 14CH4 indicates greater anthropogenic fossil CH4 emissions. *Nature*. **578**, 409–412 (2020).

40. W. Steffen, K. Richardson, J. Rockström, S. E. Cornell, I. Fetzer, E. M. Bennett, R. Biggs, S. R. Carpenter, W. de Vries, C. A. de Wit, C. Folke, D. Gerten, J. Heinke, G. M. Mace, L. M. Persson, V. Ramanathan, B. Reyers, S. Sörlin, Planetary boundaries: Guiding human development on a changing planet. *Science*. **347**, 1259855 (2015).

41. Bureau of Economic Analysis, US Leontief inverse of input-output matrix (2021), (available at https://apps.bea.gov/industry/xls/io-annual/IxI_TR_2007_2012_PRO_DET.xlsx).

42. e-stat, Japan’s Leontief inverse of input-output matrix (2015), (available at https://www.e-stat.go.jp/stat-search/file-download?statInfId=000031839469&fileKind=0).

43. A. C. H. Skelton, J. M. Allwood, The carbon price: a toothless tool for material efficiency? *Philos. Trans. R. Soc. Math. Phys. Eng. Sci.* **375**, 20160374 (2017).