Catalysing change: Defossilising the chemical industry

POLICY BRIEFING

THE ROYAL SOCIETY

Policy briefing

Politics and science frequently move on vastly different timescales. A policymaker seeking evidence on a new policy will often need the answer in weeks or months, while it takes years to design and undertake the research to rigorously address a new policy question. The value of an extended investigation into a topic cannot be understated, but when this is not possible good evidence is better than none.

The Royal Society's series of policy briefings is a mechanism aiming to bridge that divide. Drawing on the expertise of Fellows of the Royal Society and the wider scientific community, these policy briefings provide rapid and authoritative syntheses of current evidence. These briefings lay out the current state of knowledge and the questions that remain to be answered around a policy question often defined alongside a partner.

Contents

Executive summary

Society is dependent on carbon-based chemicals for everyday uses and specialist applications. The vast majority of chemicals are currently made from fossil feedstocks – oil, natural gas and coal. The chemical sector has co-developed alongside the fossil fuel industry over the last century and is currently closely integrated with, and dependent on, fossil fuels.

Whilst there will still be some fossil fuel use in 2050, there is uncertainty over the future availability and price of existing fossil feedstocks as other sectors decarbonise. The challenge this policy briefing addresses is the sourcing of alternative feedstocks, together with the science that is available to use those feedstocks and the opportunities that will be created through this evolving science.

Demand for embedded carbon in chemicals is forecast to double by 2050. Emissions will also increase if this growing demand is met with continued use of fossil feedstocks, fossil-based energy intensive production processes, and high levels of end-of-life product incineration. This will make it more difficult for society to reach net zero emissions targets and will have wider environmental implications.

The chemical sector accounts for approximately 6% of global CO_2-equivalent emissions. At least one-third of chemical sector emissions are due to direct energy consumption and chemical transformation processes, typically powered by fossil fuels. These emissions can be reduced through, for example, the electrification of power and heating and energy efficiency improvements.

The chemical sector cannot fully decarbonise, though, as most chemicals inherently contain carbon atoms that are essential to the material's structure. As this briefing explores, it could be possible to significantly 'defossilise' the organic chemical industry by replacing fossil feedstocks with alternative carbon sources, as part of the transition to a net zero chemical industry.

The alternative feedstocks explored in this briefing are biomass, plastic waste and carbon dioxide (CO_2). These can act as sources of carbon required for primary chemical building blocks, further intermediate chemicals and ultimately downstream consumer products. These alternative starting materials have the potential to reduce the chemical industry's greenhouse gas emissions.

However, the emissions and wider sustainability factors of alternative feedstocks must be carefully assessed and minimised to inform any transition. This includes the feedstock source, energy requirements for chemical transformations and production, and downstream product end-of-life treatment. It is critical that the use of alternative feedstocks does not exacerbate or lead to new environmental or societal harms.

Whilst this briefing finds that new chemistry offers many opportunities, significant challenges remain to deploying the use of alternative feedstocks at world scale production levels. This is a limiting factor on potential emissions reductions, at present. Alongside developments in chemistry, there will need to be a vast expansion of renewable energy and green hydrogen to enable the transition to a net zero chemical industry. Competition for feedstocks and energy could inhibit this transition. Long-term, cross-government, international policy coordination could help to address this risk and build in resilience of supply.

There is no single future ideal or target mix of alternative feedstocks. Biomass, plastic waste and CO_2 will likely all have a role to play in defossilising the chemical industry, but it is not possible to predict the exact future ratio of each feedstock type. This mix will change over time and space, as technologies develop, policies change, and feedstock availability and chemical industry characteristics vary between countries and commercial opportunities.

There are both challenges and opportunities of transitioning to a net zero chemical industry. There will need to be continued research and development in key fields of chemistry, such as catalysis, that are central to the advancement of many routes from alternative carbon sources to chemicals.

Without intervention, the transition to alternative feedstocks will happen over many decades. There has been progress in key areas of chemistry and the research base is growing, but there are significant technical, scientific and economic barriers to overcome for the chemical industry to transition away from fossil feedstocks to alternative carbon sources.

Alongside continued research and innovation, the question for policy and industry is how to ensure that solutions are ready for deployment and are commercially viable. This briefing identifies that competing demands for feedstock, impurity and heterogeneity of feedstock, and technology scalability are all matters that need to be resolved.

Introduction

Chemicals are ubiquitous in and essential for everyday life. This is reflected in the quantity and variety of chemicals produced worldwide: estimates of the number of commercially available chemicals range from 40,000 to over 100,000[1,2,3]. Chemicals are essential components required to produce pharmaceuticals, fertilisers, plastics, paints, adhesives, coatings, electronics, cleaning products and toiletries. Alongside these everyday commodities, chemicals are needed for essential net zero technologies, for example solar panels, wind turbines, batteries and many types of insulation.

The vast majority of chemicals upon which society relies are carbon-based. To produce carbon-based chemicals and ultimately downstream consumer products, an initial feedstock containing carbon is required.

Currently, almost 90% of feedstocks used to make chemicals are from fossil sources[4] – oil, natural gas and coal. Feedstocks are transformed, often at high temperature and pressure, into the key 'primary chemicals' used to service the chemical industry.

In this report, primary chemicals are defined as ethene (C_2H_4), propene (C_3H_6), butadiene (C_4H_6), benzene (C_6H_6), toluene ($C_6H_5CH_3$), mixed xylenes (($CH_3)_2C_6H_4$), and methanol (CH_3OH). See Section 3 for further information. These primary chemicals are transformed by a wide range of processes and chemical reactions into intermediates, speciality and fine chemicals used to make consumer products. See Figure 1 for a simplified example of the route from fossil feedstocks to consumer products. See Figure 2 for examples of uses of chemicals found in common consumer products.

FIGURE 1

Simplified example route from fossil feedstocks to a consumer product.

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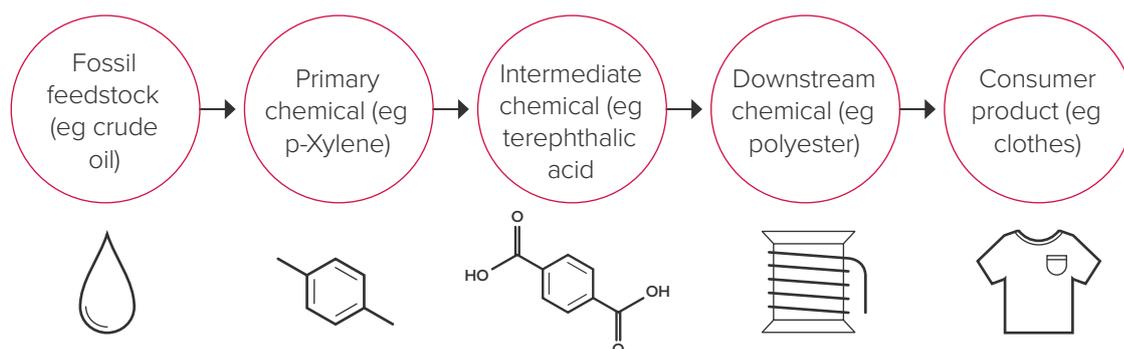
1   World Health Organization. Guidance on chemicals and health. See https://www.who.int/tools/compendium-on-health-and-environment/chemicals#:~:text=More%20than%20160%20million%20chemicals,of%20chemicals%20in%20commerce%20globally (accessed 19 February 2024).

2   UN Environment Programme. Chemical. See https://www.unep.org/beatpollution/forms-pollution/chemical

3   European Commission. Transforming EU chemicals regulation to better protect human health and the environment. See https://joint-research-centre.ec.europa.eu/jrc-news-and-updates/transforming-eu-chemicals-regulation-better-protect-human-health-and-environment-2023-12-11_en (accessed 19 February 2024).

4   Renewable Carbon Initiative. 2023. RCI carbon flows report – Compilation of supply and demand of fossil and renewable carbon on a global and European level. See https://renewable-carbon.eu/publications/product/the-renewable-carbon-initiatives-carbon-flows-report-pdf/ (accessed 19 February 2024).

FIGURE 2

Examples uses of chemicals in everyday life.
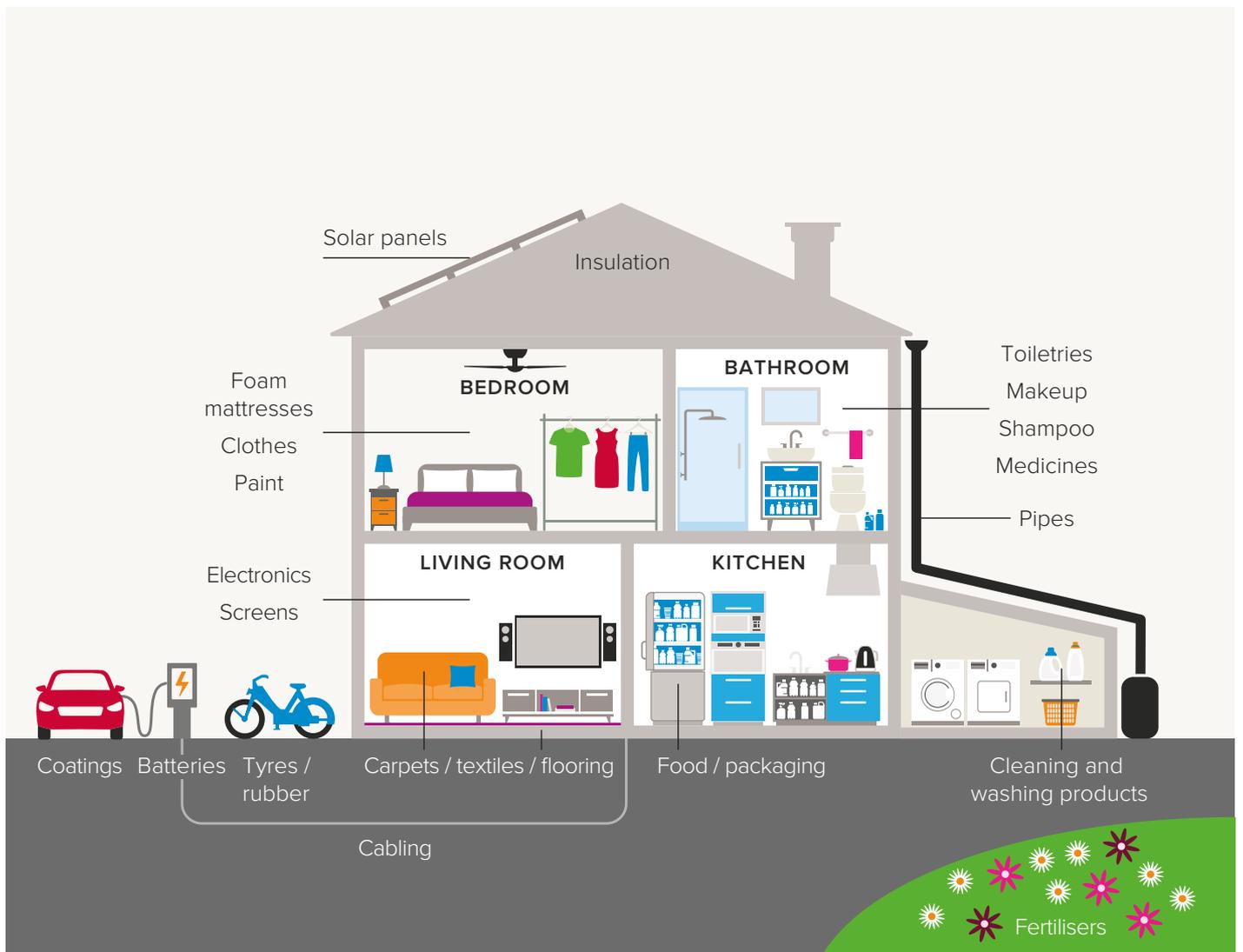
Solar panels

Insulation

Foam mattresses

Clothes

Paint

BEDROOM

BATHROOM

Toiletries

Makeup

Shampoo

Medicines

Pipes

Electronics

Screens

LIVING ROOM

KITCHEN

Coatings   Batteries   Tyres / rubber

Carpets / textiles / flooring

Food / packaging

Cleaning and washing products

Cabling

Fertilisers

The chemical sector is responsible for approximately 6% of global CO_2-equivalent emissions[5,6,7,8,9,10]. These can be categorised into Scope 1, Scope 2 and Scope 3 emissions. Estimates of chemical sector Scope 3 emissions (see Box 1) range from approximately just over one-third[11] to two-thirds[12,13] of total emissions. This briefing will use a conservative estimate of Scope 3 being responsible for approximately one-third of total emissions.

Scope definitions

Scope 1: direct emissions associated with the processes involved in making the carbon-based chemical. This includes emissions related to the combustion of fossil fuels to produce energy as well as direct process emissions.

Scope 2: upstream indirect emissions associated with purchased electricity for chemical conversion processes.

Scope 3: indirect emissions associated with upstream and downstream processes. Upstream processes include the extraction and production of feedstocks. Downstream processes include product use and end-of-life disposal, such as degradation and incineration.

5   Dhakal S *et al*. 2022 Emissions trends and drivers. In IPCC Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change. See https://www.ipcc.ch/report/ar6/wg3/downloads/report/IPCC_AR6_WGIII_Chapter02.pdf (accessed 19 February 2024).

6   World Resources Institute. 4 charts explain greenhouse gas emissions by countries and sectors. See https://www.wri.org/insights/4-charts-explain-greenhouse-gas-emissions-countries-and-sectors (accessed 19 February 2024).

7   Isella A and Manca D. 2022 GHG Emissions by (Petro)Chemical Processes and Decarbonization Priorities—A Review. Energies. **15.** See https://www.mdpi.com/1996-1073/15/20/7560 (accessed 19 February 2024).

8   Gabrielli P *et al*. 2023 Net-zero emissions chemical industry in a world of limited resources. One Earth. **6**. 682-704. See https://www.sciencedirect.com/science/article/pii/S2590332223002075 (accessed 19 February 2024).

9   S&P Global. Decarbonizing chemicals Part One: Sectorwide challenges will intensify beyond 2030. See https://www.spglobal.com/esg/insights/featured/special-editorial/decarbonizing-chemicals-part-one-sectorwide-challenges-will-intensify-beyond-2030 (accessed 19 February 2024).

10   Lange J.P. 2021 Towards circular carbo-chemicals – the metamorphosis of petrochemicals. Energy Environ. Sci. **14.** 4358-4376. See https://pubs.rsc.org/en/content/articlehtml/2021/ee/d1ee00532d (accessed 19 February 2024).

11   Bauer F. *et al*. 2022 Petrochemicals and Climate Change: Tracing Globally Growing Emissions and Key Blind Spots in a Fossil-Based Industry. Lund University Publications. See https://lup.lub.lu.se/search/publication/13c26fdd-2986-4681-ab05-f8cf0fc0f5fd (accessed 19 February 2024).

12   Renewable Carbon Initiative. CO_2 reduction potential of the chemical industry through CCU. See https://renewable-carbon-initiative.com/wp-content/uploads/2022/05/22-05-03-CO2_Reduction_Potential_of_the_Chemical_Industry_Through_CCU.pdf (accessed 19 February 2024).

13   Centre for Global Commons. Systemiq. 2022 Planet positive chemicals. See https://www.systemiq.earth/wp-content/uploads/2022/09/Main-report-v1.20-2.pdf (accessed 19 February 2024).

Chemical sector emissions are being addressed through both voluntary and regulatory means. More than 70 countries plus the EU have set targets in legislation or policy to achieve net zero emissions[14], whilst 194 countries have signed the Paris Agreement to limit global temperature increase to well below 2°C[15]. There are also chemicals-specific sustainability strategies[16], as well as industry initiatives to reduce emissions[17,18,19] in response to legislation and consumer expectations.

The chemical sector will be able to reduce Scope 1 emissions through energy efficiency improvements and by decarbonising energy-intensive processes, such as through electrification and the use of green hydrogen. However, this will not address the chemical sector's significant Scope 3 emissions associated with the extraction, processing and transportation of fossil feedstocks, as well the end-of-life emissions if downstream products are incinerated. To address this proportion of emissions, the chemical sector will have to transition to alternative sources of carbon that do not involve the extraction of fossil resources.

This policy briefing explores the feasibility and availability of three alternative sources of carbon: biomass, plastic waste and CO_2. The briefing also considers opportunities for novel processes to produce chemical products from alternative carbon sources.

14   Net Zero Tracker. 2023 Net zero stocktake 2023. See https://ca1-nzt.edcdn.com/Reports/Net_Zero_Stocktake_2023.pdf?v=1689326892 (accessed 19 February 2024).

15   United Nations Framework Convention on Climate Change. 2015 The Paris Agreeement. See https://unfccc.int/sites/default/files/resource/parisagreement_publication.pdf (accessed 15 April 2024).

16   European Chemicals Agency. Chemicals strategy for sustainability https://echa.europa.eu/hot-topics/chemicals-strategy-for-sustainability#:~:text=The%20strategy%20is%20part%20of,safer%20and%20more%20sustainable%20chemicals (accessed 19 February 2024).

17   World Economic Forum. Low-carbon emitting technologies initiative. See https://initiatives.weforum.org/low-carbon-emitting-technologies-initiative/home (accessed 19 February 2024).

18   Chemical Industries Association. UK chemical industry accelerates in race to net zero. See https://www.cia.org.uk/Media-Centre/Details/UK-chemical-industry-accelerates-in-race-to-net-zero (accessed 19 February 2024).

19   S&P Global. Decarbonizing chemicals Part One: Sectorwide challenges will intensify beyond 2030. See https://www.spglobal.com/esg/insights/featured/special-editorial/decarbonizing-chemicals-part-one-sectorwide-challenges-will-intensify-beyond-2030 (accessed 19 February 2024).

Overview of current key chemicals and their production process

Currently, around 90% of the feedstocks for the chemical industry originate from fossil sources[20], specifically, oil, natural gas and coal. Oil can be processed for ethene, propene, benzene, toluene and mixed xylenes. Natural gas and coal are used to produce ammonia and methanol. In recent years, natural gas-derived feedstocks have become much more significant for ethene and propene production, due to the rise in shale gas production in, for example, the US[21].

Whilst ammonia is also considered a primary chemical, it is not addressed in this report, as it is not a carbon-based chemical and was recently the subject of a Royal Society report[22]. It is important to note that ammonia is one of the largest drivers of chemical sector emissions, accounting for almost 2% of global carbon dioxide emissions[23].

The vast range of final products currently rely on these primary chemicals[24,25]. Collectively, primary chemicals account for two thirds of the global energy demand of the chemical sector[26] and underpin many thousands of chemical products. However, the future chemical industry does not necessarily have to follow this linear structure dominated by primary chemicals. Biomass and plastic waste carbon feedstocks could generate new or different primary chemicals than those used today, though may also offer opportunities to bypass primary chemicals and develop new pathways more directly to fine or speciality chemicals.

Other feedstocks that are important for the chemical industry include water, oxygen, nitrogen, hydrogen, and the halogens (chlorine, bromine and iodine), although these are not the focus of this briefing.

A broad overview of how fossil fuel feedstocks are currently processed, firstly into primary chemicals and then into the everyday products on which society relies is shown in Figure 3.

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20 Renewable Carbon Initiative. *Op. cit*.

21 National Academies of Sciences, Engineering and Medicine. 2016 The changing landscape of hydrocarbon feedstocks for chemical production: Implications for catalysis: Proceedings of a workshop. See https://www.nationalacademies.org/our-work/the-changing-landscape-of-hydrocarbon-feedstocks-for-chemical-production-implications-for-catalysis-proceedings-of-a-workshop (accessed 15 March 2024).

22 Royal Society. 2020 Ammonia: Zero-carbon fertiliser, fuel and energy store. See https://royalsociety.org/news-resources/projects/low-carbon-energy-programme/green-ammonia/ (accessed 15 March 2024).

23 *Ibid*.

24 Meng F *et al*. 2023 Planet-compatible pathways for transitioning the chemical industry. PNAS. **120.** See https://www.pnas.org/doi/10.1073/pnas.2218294120 (accessed 19 February 2024).

25 Centre for Global Commons. Systemiq. *Op. cit*.

26 International Energy Agency. 2018 The future of petrochemicals. See https://iea.blob.core.windows.net/assets/bee4ef3a-8876-4566-98cf-7a130c013805/The_Future_of_Petrochemicals.pdf (accessed 19 February 2024).

FIGURE 3

Simplified flow diagram showing the production of end-use applications and consumer products from fossil feedstocks.

Fossil feedstocks	Crude oil		Natural gas	Coal
Refining and processing	Ethane	Propane	Butanes	Naphtha	Syngas
Primary chemicals	Ethene	Propene	Butadiene	Benzene / Toluene / Xylenes	Methanol
Intermediate chemicals	Monomers, polymers, pharmaceutical intermediates				
End-use applications and consumer products	Plastics / Elastics	Insulation / Coatings	Paints / Electronics	Tyres / Adhesives	Medicines / Textiles

The manufacture and use of the primary chemicals are described below.

1.1 Ethene
Ethene is primarily produced by the steam cracking of ethane (see Box 2), which is largely a product of natural gas processing, or naphtha, which is a product of crude oil distillation. Approximately 170 million tonnes (Mt) of ethene is produced globally every year[27]. The majority of ethene is used to produce a range of polymers which include high density polyethylene (HDPE), low density polyethylene (LDPE), linear low density polyethylene (LLDPE), polyethylene terephthalate (PET), polyvinylchloride (PVC), and polystyrene (PS). All of these polymers are used widely for clothing fibres, plastic packaging, film, pipes and bottles.

1.2 Propene
Propene is mainly produced by the steam cracking process from either naphtha or propane. It is also a by-product of petroleum refining. Production of propene via propane dehydrogenation and the methanol-to-olefins process is also becoming increasingly important.

Approximately 130 Mt of propene is produced globally every year[28]. Major uses for propene include polypropylene (PP), polyurethanes (via propylene oxide and polyols), acetone (via cumene), acrylonitrile for polymer applications, and polymethylacrylates (via acrylic acid).

These products are found in a wide variety of downstream chemical products and end uses, for example in polyurethanes for insulation, coatings and adhesives[29], whilst acetone is used widely in paints, solvents, nail varnish remover and adhesives[30].

1.3 Butadiene
Butadiene is produced via steam cracking of naphtha, with approximately 18 Mt being produced globally each year, making it the least-produced olefin. It has applications in a wide variety of specialised products such as styrene-butadiene rubber (SBR), polybutadiene rubber (PBR), nitrile rubbers (NBR), adiponitrile (mainly used as the starting point for nylon-66), acrylonitrile-butadiene-styrene resins (ABS) and thermoplastic elastomers.

1.4 Benzene
Approximately 55 Mt of benzene is produced annually[31] via oil refining or from steam cracking of naphtha. Benzene is used to produce polystyrene (via ethylbenzene), cumene, cyclohexane and nitrobenzene.

The value chain for benzene is shown schematically in Figure 4 (overleaf) and demonstrates the complexity and interconnectedness of the chemical industry.

27 Isella A and Manca D. 2022 GHG Emissions by (Petro)Chemical Processes and Decarbonization Priorities—A Review. Energies. **15.** See https://www.mdpi.com/1996-1073/15/20/7560 (accessed 19 February 2024).

28 *Ibid*.

29 de Souza F, Pawan K, Gupta R. 2021 Introduction to polyurethane chemistry. In: Gupta R and Kahol K (eds.) Polyurethane chemistry: Renewable polyols and isocyanates. Pittsburg, Kansas, USA: ACS Publications. See https://pubs.acs.org/doi/10.1021/bk-2021-1380.ch001#:~:text=Polyurethanes%20are%20an%20immensely%20versatile,diisocyanate%20polyaddition%20reactions%20by%20Dr (accessed 19 February 2024).

30 Public Health England. Acetone: general information. See https://www.gov.uk/government/publications/acetone-properties-and-incident-management/acetone-general-information (accessed 19 February 2024).

31 Isella and Manca. *Op. cit*.

BOX 2

Steam cracking

Steam cracking is a process in which a hydrocarbon feedstock, such as ethane, propane or naphtha is converted to olefins (ethene, propene and butadiene). The raw material input is 'cracked' in high temperature furnaces in the presence of steam. Typically, to achieve the high temperatures required – in the range of 800 – 1,000°C – significant quantities of fuel, such as methane, are burned. This leads to significant CO_2 emissions, in the range of 0.5 – 1.5 tonnes of CO_2 per tonne of olefin product, depending on the feedstock used.

The cracking reactions occur very rapidly, in the order of fractions of a second. The range of products that are obtained depend on the feed composition, the hydrocarbon to steam ratio and on the temperature of the furnace. Lighter hydrocarbon feeds, such as ethane or liquified petroleum gas, will crack to give light olefins (ethene, propene and butene) as products. Cracking of heavier, liquid feeds such as naphtha, will give aromatic hydrocarbons as well as olefins.

A modern steam cracker is a large plant with a high degree of heat integration that can have the capability of producing more than 1.5 Mt of olefins each year. As such, steam cracking is the core technology for producing large quantities of many primary chemicals. A facility of this size can cost around USD $2 – 5 billion[32,33,34].

32   S&P Global. Enterprise planning new 2 mil mt/year steam cracker in Texas: documents. See https://www.spglobal.com/commodityinsights/en/market-insights/latest-news/chemicals/061522-enterprise-planning-new-2-mil-mtyear-steam-cracker-in-texas-documents (accessed 19 February 2024).

33   TotalEnergies. United States: TotalEnergies announces the start-up of New Ethane Cracker in Port Arthur. See https://totalenergies.com/media/news/press-releases/united-states-totalenergies-announces-start-new-ethane-cracker-port (accessed 19 February 2024).

34   Hydrogen Central. INEOS secures £3.1bn to build Europe's greenest 'cracker' powered by hydrogen. See https://hydrogen-central.com/ineos-secures-3-1bn-build-europes-greenest-cracker-powered-hydrogen/ (accessed 19 February 2024).

FIGURE 4

Simplified flow diagram displaying the route from fossil feedstocks to benzene to end products, highlighting the complexity of the chemical industry.

KEY

- Methanol
- Ethene
- Propene
- Butadiene

Crude oil		Polystyrene	Cups insulation, food service / packaging
	Ethylbenzene → Styrene	ABS resins	Auto parts, consumer electronics
		SAN resins	Housewares, appliances parts, cosmetic packaging
		SB latex	Carpet backing, paper coating
Benzene		SB rubber	Tyres, adhesives
Coal	Cumene → Phenol	PF resins	Wood adhesives
	Cumene → BPA	Epoxy resins, polycarbonates	Coatings, medical
	Cumene → Acetone	MMA	Automotive panels, medical equipment, baseball helmets
	Nitrobenzene → Aniline	MDI	
		Rubber chemicals	
		Dyes, pigments	
		Herbicides	
	Cyclohexane		Nylon fibres

ABS resins = Acrylonitrile-Butadiene-Styrene resins   SAN resins = Styrene acrylonitrile resin   SB latex = Styrene-Butadiene Latex
SB rubber = Styrene-butadiene rubber   PF resins = Phenol formaldehyde resins   MMA = Methyl methacrylate   BPA = bisphenol A
MDI = Methylene diphenyl diisocyanate

1.5 Toluene and mixed xylenes

Toluene and xylenes are also produced via oil refining or from the steam cracking of naphtha, with approximately 29 Mt of toluene[35] and 70 Mt of xylenes being produced annually. The majority of toluene ends up in the petrol pool to be used as fuel. Other uses of toluene include benzene and xylene production (via disproportionation), toluene di-isocyanate for manufacture of polyurethanes, and solvents.

The primary chemical application for xylenes is in the manufacture of PET, for which para-xylene is the feedstock. Benzene, toluene and mixed xylenes are collectively known as BTX.

1.6 Methanol

In many countries, methanol is predominantly produced from syngas – a mixture of hydrogen, carbon monoxide and CO_2 – produced by steam reforming of natural gas, shown in Box 3. Methanol can also be produced via coal gasification. This is the primary production route in China[36], which is the largest methanol producer in the world[37]. Approximately 100 Mt of methanol is produced globally each year[38]. Methanol is an important intermediate in the manufacture of a wide variety of downstream chemical products, including formaldehyde, acetic acid and solvents. Methanol is also finding increasing application in the manufacture of ethene and propene via the methanol-to-olefins (MTO) process and as a fuel.

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35 Isella and Manca. *Op. cit*.

36 International Energy Forum. Here's why China is betting big on methanol. See https://www.ief.org/news/heres-why-china-is-betting-big-on-methanol (accessed 19 February 2024).

37 International Renewable Energy Agency. 2021 Innovation outlook: Renewable methanol.
    See https://www.irena.org/-/media/Files/IRENA/Agency/Publication/2021/Jan/IRENA_Innovation_Renewable_Methanol_2021.pdf (accessed 19 February 2024).

38 *Ibid*.

BOX 3

Steam reforming

Steam reforming is the method where hydrocarbon feedstock (such as methane) and steam are converted to syngas. The process, which operates at high temperatures in the range 650 – 950°C using a nickel catalyst, can be described by the following reaction:

$$CH_4 + H_2O \rightleftharpoons 3\,H_2 + CO$$

Furthermore, carbon monoxide also reacts with steam via the water-gas shift reaction to produce additional hydrogen and CO_2:

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

The main application of steam reforming is the production of hydrogen, with more than 60% of the world's current hydrogen needs being produced via steam reforming of natural gas[39]. Around 60% of the hydrogen used in industry is for ammonia production[40].

Syngas produced via steam reforming is also used to produce methanol, as well as liquid hydrocarbons (via Fischer-Tropsch synthesis). These applications account for roughly 20% of global hydrogen production.

39 International Energy Agency. 2023 Global hydrogen review. See https://iea.blob.core.windows.net/assets/ecdfc3bb-d212-4a4c-9ff7-6ce5b1e19cef/GlobalHydrogenReview2023.pdf (accessed 19 February 2024).

40 *Ibid.*

Reasons to replace fossil carbon in chemical products

2.1 Current chemical sector emissions
The main driver to replace fossil feedstocks with alternative carbon sources is the scale of the chemical sector's emissions.

Considering Scope 1, 2 and 3 emissions, the chemical sector is responsible for approximately 6% of global CO_2-equivalent emissions. The sources of Scope 1, 2 and 3 emissions in the chemical sector are shown in Figure 5.

FIGURE 5

Sources of chemical sector Scope 1, 2 and 3 emissions.

Scope 1 emissions
Direct emissions associated with the processes involved in making the carbon-based chemical. This includes emissions related to the combustion of fossil fuels to produce energy as well as direct process emissions.

Scope 2 emissions
Upstream indirect emissions associated with purchased electricity for chemical conversion processes.

Scope 3 emissions
Indirect emissions associated with upstream and downstream processes. Upstream processes include the extraction and production of feedstocks. Downstream processes include product use and end-of-life disposal, such as degradation and incineration.
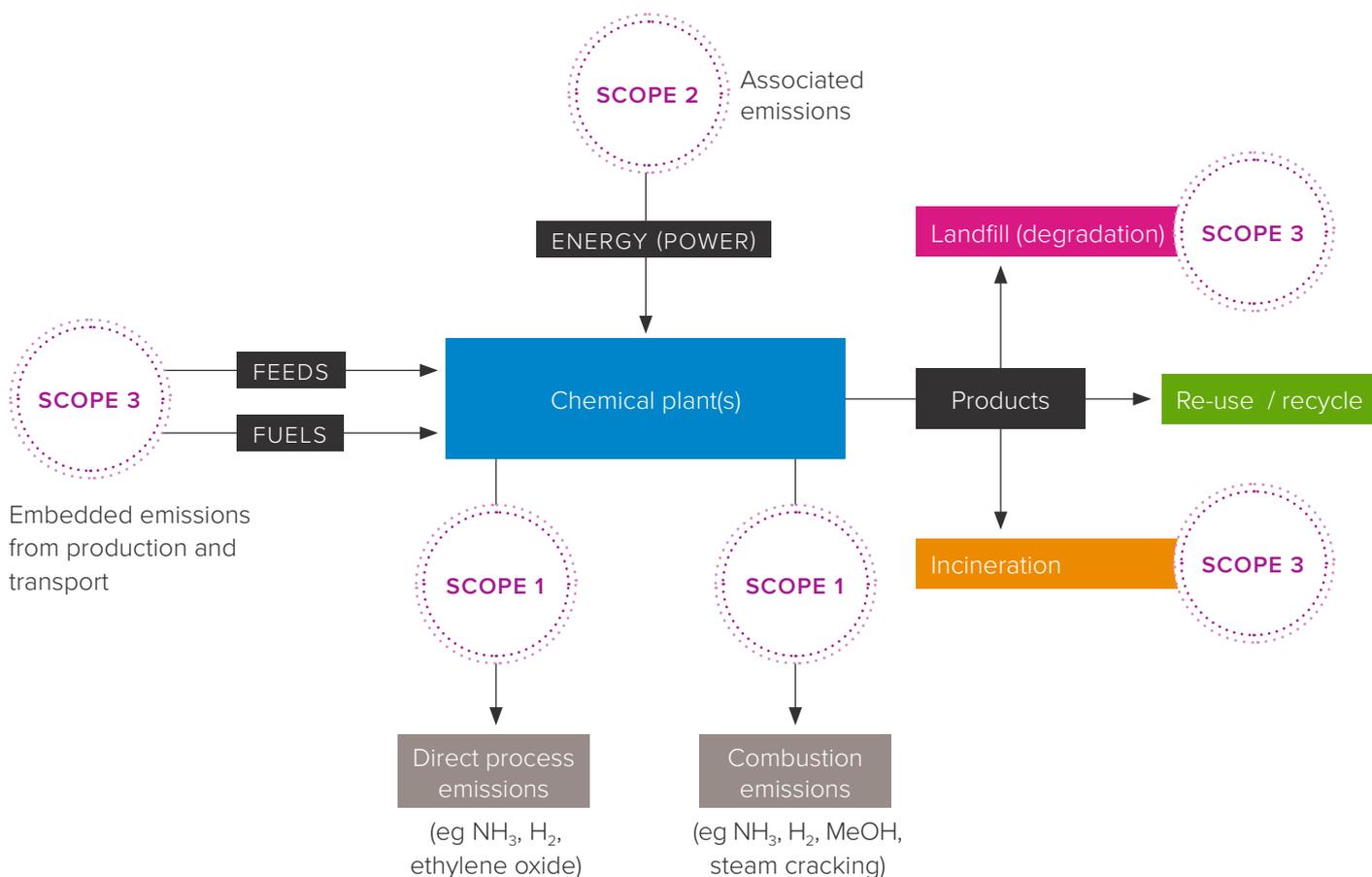
The main energy demands of the chemical industry, which are responsible in large part for its Scope 1 emissions, are to facilitate the key transformation processes of fossil feedstocks into chemicals. These processes include steam reforming, gasification, steam cracking, fluid catalytic cracking, catalytic reforming, and distillation and compression processes. To meet net zero targets and reduce chemical sector emissions, it will be critical to reduce the substantial fossil fuel use for direct energy consumption in chemical manufacturing processes.

Fossil fuel use for direct energy consumption could be reduced through measures such as energy efficiency, electrification, and the use of electrolytic green hydrogen. There are costs and carbon emissions associated with the implementation of equipment and infrastructure for each of these, which must be considered as part of a broader sustainability evaluation. In particular, the additional hydrogen required will have to be produced using renewable energy to ensure it has lower emissions. Electrification of systems poses huge challenges to current production methods, as, for example, it is not currently possible to electrify a steam cracker or steam methane reformer given the scale of energy demand. Scope 1 emissions must be addressed to achieve a net zero chemical sector and the routes to doing so will need consideration and investment.

However, it is also important to address Scope 3 emissions associated with the embedded carbon in the initial feedstock used to make chemicals. Estimates of chemical sector Scope 3 emissions range from approximately just over one-third[41] to two-thirds[42,43,44] of total emissions. This briefing will use the lower end of this range, assuming that Scope 3 is responsible for approximately one-third of total emissions.

Scope 3 emissions are tied to the use of oil, gas and coal as raw materials in the industry. There is currently approximately 550 Mt per year of embedded carbon in feedstocks for chemicals and derived material. An estimated 88% of this is fossil-based, 8% bio-based, 4% recycled, and less than 0.1% is from CO_2. Demand for embedded carbon could be approximately double, at over 1.1 Gt, by 2050[45].

41 Bauer *et al*. *Op. cit*.

42 Renewable Carbon Initiative. CO_2 reduction potential of the chemical industry through CCU. See https://renewable-carbon-initiative.com/wp-content/uploads/2022/05/22-05-03-CO2_Reduction_Potential_of_the_Chemical_Industry_Through_CCU.pdf (accessed 19 February 2024).

43 Centre for Global Commons. Systemiq. *Op. cit*.

44 McKinsey. Sustainable feedstocks: Accelerating recarbonization in chemicals. See https://www.mckinsey.com/industries/chemicals/our-insights/sustainable-feedstocks-accelerating-recarbonization-in-chemicals (accessed 19 February 2024).

45 Renewable Carbon Initiative. 2023. *Op. cit*.

2.2 Fossil feedstock uncertainty

Fossil feedstocks for the manufacture of chemical products are almost always co-products of wider hydrocarbon use. At present, approximately 10% of all global fossil carbon[46] is used by the chemical industry as feedstock.

The global share of fossil fuels as a primary energy source has been projected to fall from 80% in 2019 to between 55 and 20% by 2050[47]. As fossil use for transport and power declines, the proportion of fossil carbon being used by the chemical industry compared to other sectors will increase – if the sector continues to rely on fossil feedstocks[48].

As chemical industry demand for fossil carbon increases and energy and transport sector demand decreases, some estimate that the chemical industry could have the same demand for embedded carbon as energy and transport by 2050[49]. It should be noted, though, that there is uncertainty over this as changing economic, policy and societal drivers in each sector will influence demand for fossil carbon.

As fossil use in other sectors declines, there may be greater availability of fossil feedstocks for the chemical industry in the short- to medium-term[50]. There is growing interest in refinery operations switching focus to supply petrochemical feedstocks to reflect changing demand[51]. However, in the longer term, the chemical industry may have to pay an increasing portion of the cost of oil processing to prepare fossil feedstocks, leading to rising costs. In addition, if CO_2 emissions pricing rise the costs of fossil feedstocks will increase further.

There is uncertainty around the long-term cost of fossil feedstocks, as petrochemical infrastructure investments and supply and demand changes. Further research on these economic influences could be helpful for policy and industry decision makers to ensure resilience of supply chains from chemical manufacturers to downstream users and citizen consumers.

46 Renewable Carbon Initiative. 2022 Renewable carbon as a guiding principle for sustainable carbon cycles. See https://renewable-carbon.eu/publications/product/renewable-carbon-as-a-guiding-principle-for-sustainable-carbon-cycles-pdf/ (accessed 19 February 2024).

47 BP Energy Outlook 2023 https://www.bp.com/content/dam/bp/business-sites/en/global/corporate/pdfs/energy-economics/energy-outlook/bp-energy-outlook-2023.pdf

48 Lopez G, Keiner D, Koiranen T, Breyer C. 2023 From fossil to green chemicals: sustainable pathways and new carbon feedstocks for the global chemical industry. Energy Environ. Sci. **16.** 2879-2909. See https://pubs.rsc.org/en/content/articlehtml/2023/ee/d3ee00478c (accessed 20 February 2024).

49 Renewable Carbon Initiative. 2022. *Op. cit*.

50 Lange. *Op. cit.*

51 International Energy Agency. 2023 Oil. See https://iea.blob.core.windows.net/assets/6ff5beb7-a9f9-489f-9d71-fd221b88c66e/Oil2023.pdf (accessed 19 February 2024).

Biomass as a feedstock for chemicals

3.1 Types of biomass

Biomass can be considered as "material of biological origin excluding material embedded in geological formations and/or fossilised"[52]. The types of biomass covered by this definition include: biomass crops; food crops, such as vegetable oils and starches; agricultural residues; forest residues; horticultural residues; marine biomass; municipal food and garden waste and the biogenic fraction of municipal waste, such as paper and card.

Biomass has a highly heterogeneous nature, as the biomass composition depends on the plant species, location and year-to-year variability. Dry plant matter is known as lignocellulosic biomass. This is made of polysaccharide carbohydrates – cellulose and hemicelluloses – and an aromatic polymer, lignin[53]. Lignin makes plant cell walls, accounting for approximately one-third of lignocellulosic biomass[54].

Image:
Biogas plant behind corn field.
© iStock.com / marvinh.

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52 European Commission. Biomass. See https://knowledge4policy.ec.europa.eu/glossary-item/biomass_en (accessed 20 February 2024).

53 Zoghlami A, Paës G. 2019 Lignocellulosic biomass: Understanding recalcitrance and predicting hydrolysis. Front. Chem. **7.** See https://www.frontiersin.org/articles/10.3389/fchem.2019.00874/full (accessed 13 March 2024).

54 Tang D, Huang Z, Tang W, Jin Y. 2021 Lignin-to-chemicals: Application of catalytic hydrogenolysis of lignin to produce phenols and terephthalic acid via metal-based catalysts. International Journal of Biological Macromolecules. **190.** 72-85. See https://www.sciencedirect.com/science/article/abs/pii/S0141813021018626 (accessed 13 March 2024).

3.2 Biomass to chemicals processes

Processes that can be used for the conversion of biomass products to chemicals are either thermochemical, such as direct gasification, or thermo-catalytic and bio-catalytic, such as hydrolysis. Thermochemical processing is used to convert biomass into products such as biochar, bio-oil and syngas. Biochar and bio-oil contain corrosive and unstable oxygenates and are therefore difficult to use.

Enabling these to be valuable products for the chemical industry is an active area of research. A promising conversion method is the direct gasification of biomass at high temperatures (>700°C) and low oxygen levels to produce a syngas mixture containing hydrogen, carbon monoxide, CO_2 and methane[55]. Another thermochemical route is pyrolysis – see Box 4.

BOX 4

Biomass pyrolysis

Pyrolysis uses thermal degradation to convert feedstocks into solid, liquid and gaseous products. The products formed are heavily dependent on the composition of the feedstock in question and process conditions. The type of reactor, heat transfer, residence time, heating rate and temperature all impact product formation[56].

Oxygen contained within the structural components of biomass – lignin, cellulose and hemicellulose – leads to pyrolysis oils. These oils contain oxygenated compounds that can be detrimental to oil stability and lead to undesirable properties. Catalytic pyrolysis has advantages over non-catalytic pyrolysis[57], as it reduces the activation energy of feedstock degradation and provides control over product formation, helping to increase the purity, directing towards higher value products, and promoting the removal of oxygen from pyrolysis oils[58].

Developments to catalytic pyrolysis seek to improve selectivity, promote deoxygenation reactions and reduce catalyst degradation through coke formation. This is a major challenge for commercial catalytic pyrolysis[59]. Commercial operations usually seek valorisation through production of biochar or crude pyrolysis oils that can be used directly as fuels, as feedstocks in fuel production, or as feedstocks for production of other materials and chemicals. It is also possible to valorise the gaseous products, but these are often combusted to provide process heat.

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55 Osman A, Mehta N, Elgarahy A, Al-Hina A, Al-Muhtaseb A, Rooney D. 2021 Conversion of biomass to biofuels and life cycle assessment: a review. Environmental Chemistry Letters. See https://link.springer.com/article/10.1007/s10311-021-01273-0 (accessed 20 February 2024).

56 Yogalakshmi KN *et al.* 2022 Lignocellulosic biomass-based pyrolysis: A comprehensive review. Chemosphere. **286.** See https://www.sciencedirect.com/science/article/abs/pii/S0045653521022967 (accessed 14 March 2024).

57 *Ibid.*

58 Nishu *et al.* A review on the catalytic pyrolysis of biomass for the bio-oil production with ZSM-5: Focus on structure. Fuel Processing Technology. **199.** See https://www.sciencedirect.com/science/article/abs/pii/S0378382019313451 (accessed 14 March 2024).

59 Eschenbacher A, Fennell P, and Jensen AD. A review of recent research on catalytic biomass pyrolysis and low-pressure hydropyrolysis. Energy Fuels. **35.** 18333–18369. See https://pubs.acs.org/doi/abs/10.1021/acs.energyfuels.1c02793 (accessed 14 March 2024).

Biochemical processing, such as hydrolysis and fermentation, leads to chemical compounds such as adipic acid, glycerol, fumaric acid and propylene glycol. These can be widely used for pharmaceutical, polymers, cosmetics, solvents and broader chemical products[60,61]. This offers the opportunity to bypass the existing primary chemicals stage, which is beneficial in terms of energy use and manufacturing complexity.

Biomass-sourced carbon is more oxidised than all components of fossil carbon. This means that commodity chemicals with oxygen atoms in their structure require fewer processing steps to be produced from biomass than fossil feedstocks. This could be a potential advantage over fossil feedstocks. However, much further research and development is required into known and potentially viable routes to converting oxygenates into valuable chemicals. More research is also needed into addressing disadvantages such as high water content, lower energy content and removing impurities.

In contrast, the production of conventional building blocks with no oxygen atoms, such as ethene, from biomass is energy intensive as it requires its deoxygenation. This could encourage the production of novel chemical building blocks from biomass that are closer to the final products – bypassing the existing dominant primary chemicals. This may theoretically mean the future chemical industry manufactures many more final products, rather than deriving the majority of products from just a few primary chemical building blocks.

Further research is required to better understand any potential technical and economic implications of a less integrated value chain. This ambition requires the development of novel chemical transformations with the potential of having fewer processing steps and lower energy demands than current ones. A potential example of this is shown in Box 5.

60 Straathof A, Bampouli A. 2017 Potential of commodity chemicals to become bio-based according to maximum yields and petrochemical prices. Biofpr. **11.** 798-810. See https://onlinelibrary.wiley.com/doi/10.1002/bbb.1786 (accessed 20 February 2024).

61 US Department of Energy. 2004 Top Value Added Chemicals from Biomass. See https://www.nrel.gov/docs/fy04osti/35523.pdf (accessed 20 February 2024).

BOX 5

Biomass to levulinic acid

Levulinic acid is seen as an attractive 'stepping stone' chemical building block that can be made from waste biomass[62]. Possessing two different reactive functional groups – ketone and carboxylic acid – levulinic acid is highly versatile for the synthesis of a large number of downstream intermediate chemicals[63], which are used in many industries including polymers, electronics, cosmetics, solvents and fuels.

Levulinic acid synthesis has been studied extensively in academia[64], using a wide range of biomass sources, such as food crops, food waste and even algal biomass[65]. In particular, levulinic acid can be derived from five- and six-carbon sugars, such as xylose and glucose found in lignocellulosic biomass feedstocks, including waste wood.

Levulinic acid is now being commercially produced from biomass, principally as a solvent rather than as an intermediate. Reducing the cost and energy intensity of this potentially important intermediate is the next challenge, to move beyond very small-scale production and to lower associated emissions. The downstream conversion of levulinic acid to other chemicals has attracted attention from electrochemical investigation to improve efficiencies[66].

To make any substantial impact on the emissions of the global chemical industry, routes from alternative carbon sources will have to be made as low emission as possible and replace high emission pathways at significant scale.

Biomass to levulinic acid route[67]

Biomass → Pretreatment → Polysaccharide (carbohydrates) → Monosaccharide (eg xylose and glucose) → Levulinic acid → Downstream chemicals

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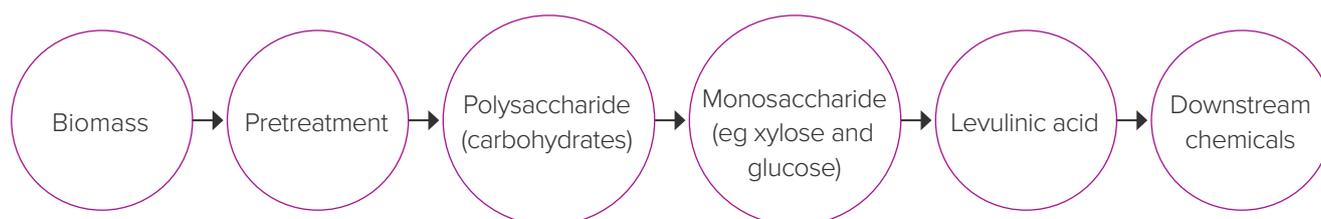
62 Maastricht University. Developing a new value chain from biomass to C6 monomers. See https://www.maastrichtuniversity.nl/research/bm2c6 (accessed 20 February 2024).

63 Renewable Carbon News. 2019 See https://renewable-carbon.eu/news/levulinic-acid-and-succinic-acid-a-realistic-look-at-the-present-and-future-of-two-versatile-bio-based-platform-chemicals-and-their-market-development/ (accessed 20 February 2024).

64 Signoretto M, Taghavi S, Ghedini E, Menegazzo F. 2019 Catalytic production of levulinic acid (LA) from actual biomass. MDPI Molecules. **24.** See https://www.mdpi.com/1420-3049/24/15/2760 (accessed 20 February 2024).

65 *Ibid.*

66 dos Santos T, Nilges P, Sauter W, Harnisch F, Schröder U. 2015 Electrochemistry for the generation of renewable chemicals: electrochemical conversion of levulinic acid. RSC Advances. **34.** See https://pubs.rsc.org/en/content/articlelanding/2015/ra/c4ra16303f (accessed 20 February 2024).

67 Signoretto *et al. Op cit.*

3.3 Biomass availability

There are many complex, interacting factors that will influence the future availability of biomass. These include improvements in crop yields (itself connected to the production of energy intensive fertilisers), the impact of climate change on agricultural productivity, the extent to which productive agricultural land is used for food or biomass crop cultivation, future global population and dietary change, demand for biofuels, and the protection of land for nature. Biomass availability will differ between countries and regions, due to a range of factors including geography and domestic policy.

Approximately 60 EJ (exajoules) of solid bioenergy (energy generated from biomass) is used per year globally[68,69]. This is equivalent to around 4.3 Gt of fresh biomass[70]. Under future net zero scenarios which account for food supply and environmental considerations, estimates of the future bioenergy supply required range from 85 – 250 EJ per year[71,72]. Using the assumption from the International Energy Agency of 100 EJ per year[73], this equates to just over 7 Gt of biomass, including moisture content.

However, there are many potential uses for biomass, with competing sectoral demands, such as for food, animal feed and bioenergy.

For example, global food production may have to increase by more than 50% by 2050 to meet demands for a growing population[74,75], whilst demand for bioenergy has risen by 3% per year since 2010 and is forecast to continue increasing[76]. There is also increasing demand for biomass for Sustainable Aviation Fuels (SAF) – see Case Study 1.

68 International Energy Agency. 2022 World Energy Outlook 2022. See https://iea.blob.core.windows.net/assets/830fe099-5530-48f2-a7c1-11f35d510983/WorldEnergyOutlook2022.pdf (accessed 19 February 2024).

69 Dhakal *et al. Op. cit*.

70 Centre for Global Commons. Systemiq. *Op. cit*.

71 Climate Change Committee. 2018 Biomass in a low-carbon economy. See https://www.theccc.org.uk/wp-content/uploads/2018/11/Biomass-in-a-low-carbon-economy-CCC-2018.pdf (accessed 19 February 2024).

72 Dhakal *et al. Op. cit*.

73 International Energy Agency. 2022. *Op. cit*.

74 van Dijk M, Morley T, Rau M, Saghai Y. 2021 A meta-analysis of projected global food demand and population at risk of hunger for the period 2010–2050. Nature Food. **2.** 494-501. See https://www.nature.com/articles/s43016-021-00322-9 (accessed 19 February 2024).

75 World Resources Institute. 2018 How to sustainably feed 10 billion people by 2050, in 21 charts. See https://www.wri.org/insights/how-sustainably-feed-10-billion-people-2050-21-charts (accessed 19 February 2024).

76 International Energy Agency. Bioenergy. See https://www.iea.org/energy-system/renewables/bioenergy (accessed 19 February 2024).

Sustainable Aviation Fuels (SAF) biomass demand in the UK

The UK government has placed a strong emphasis on the use of biomass for sustainable aviation fuels. The UK has an upcoming SAF mandate, "requiring at least 10% (c.1.2 Mt) of jet fuel to be made from sustainable sources by 2030"[77]. At present, only a very small fraction of biofuel is used in the UK aviation sector.

However, a previous Royal Society report[78] has outlined the challenges of meeting the UK's SAF demand through biomass. The report outlines three energy crop scenarios – for oil seed rape, miscanthus and poplar – in which more than 50% of all UK agricultural land would be needed to produce the necessary amount of biomass to replace all the UK's aviation fuel. Alternatively, waste cooking oil, agricultural residues, forest residues and municipal waste could account for approximately 20% of jet fuel demand.

Alongside land use challenges associated with SAF from biomass, the emissions from the production methods and burning SAF at altitude should be considered. Whilst biomass for both chemical feedstocks and SAF used in the UK could be sourced from international markets, the above example is to illustrate the potential implications of replacing fossil sources with biomass at significant scales.

77   Department for Transport. 2022 Sustainable aviation fuels mandate. See https://assets.publishing.service.gov.uk/
media/6305fca9e90e0729d7707973/sustainable-aviation-fuels-mandate-summary-of-consultation-responses-and-
government-response.pdf (accessed 20 February 2024).

78   Royal Society. 2023 Net zero aviation fuels: Resource requirements and environmental impacts.
See https://royalsociety.org/-/media/policy/projects/net-zero-aviation/net-zero-aviation-fuels-policy-briefing.pdf
(accessed 20 February 2024).

Considering the above competing demands and wider sustainability considerations, it is unlikely that existing sources of biomass will provide a significant percentage of embedded carbon required by the chemical industry under expected growth trajectories. Biomass may, though, act as a promising route for more limited markets, such as for speciality chemicals – see section 3.5 for potential examples.

3.4 Challenges and future research needs

There are several challenges to scaling the use of biomass as a chemical feedstock. As discussed, one of the main issues to a bio-based carbon industry is that sources of biomass are limited and there is competition for these raw materials from other sectors, mainly for bioenergy but also increasingly in other sectors, such as for aviation fuels. To maximise value from potentially limited resources, the priority for research could be on new or specialist chemicals in high margin applications such as food, health and well-being products or cosmetics. However, due to their small scale in comparison to primary chemicals production, this would not make a significant contribution to the overall net zero transition.

Furthermore, biomass has a highly heterogeneous nature. Generally, chemical processes are difficult to adapt to variable feedstocks as the industry has been built largely on the use of uniform and consistent raw materials. This could cause issues for businesses if there is a significant number of highly bespoke processes for converting different biomass types to chemicals and downstream products.

One of the most difficult and pressing challenges of converting biomass to chemicals is processing lignocellulose[79]. This is heterogeneous in its structure and weight distribution, making it difficult to process. As a result, lignocellulose is often discarded as waste produc or burned for heating and power generation[80], leading to the loss of a potential biomass source for chemicals production or other uses. Research and innovation that helps make the processing of lignocellulose easier could unlock the economic value of this hugely underutilised resource for making higher value chemicals[81].

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79 Zoghlami and Paës. *Op. cit*.

80 Zhou N, Thilakarathna WPDW, He QS, Rupasinghe HPV. 2022 A review: Depolymerization of lignin to generate high-value bio-products: opportunities, challenges, and prospects. Front. Energy Res. **9.** See https://www.frontiersin.org/articles/10.3389/fenrg.2021.758744/full (accessed 14 March 2024).

81 *Ibid*.

The diverse spatial distribution of biomass sources could also pose logistical transportation or cost challenges for chemical producers[82]. Collaboration on efficient process design and technology sharing could help the sector to avoid some of these issues, whilst there could also be greater opportunities for smaller, integrated biorefineries. The use of more novel forms of biomass, such as seaweed and algae, is still at the research phase.

There is a need to develop pre-treatment technologies, including physical (which are energy intensive and require specialised equipment) and/or chemical (requiring the use of chemicals) methods depending on the specifications. As mentioned, one of the main challenges is the difficulty of processing lignocellulose and specifically separating out lignin from cellulose. The efficient pretreatment of lignocellulosic biomass will present an important breakthrough.

3.5 Emerging routes from biomass to chemicals

Biomass and bio-derived products present a valuable opportunity to be electrocatalytically converted into bespoke chemicals, such as for cosmetics and pharmaceuticals – though, again, these are not at a significant scale of production to substantially reduce chemical sector emissions in line with net zero targets. An example of an alternative plastic production route and an example of potential green hydrogen co-production[83] is outlined overleaf in Figure 6.

### 3.5.1 Glycerol to lactic acid

In 2022, around 2.3 billion litres of biodiesel were produced in the UK[84]. Glycerol is the main by-product of biodiesel production. Glycerol of high purity (>98%) can be electrocatalytically converted to high value products, such as organic acids, depending on the catalyst and the potentials applied[85]. The selectivity to such products is difficult to control and so is the separation of such mixtures from the aqueous phase.

82 Abu-Omar M. and Ford P. 2023 The lignin challenge in catalytic conversion of biomass solids to chemicals and fuels. RSC Sustain. **1.** 1686-1703. See https://pubs.rsc.org/en/content/articlelanding/2023/su/d3su00117b#:~:text=Particular%20emphasis%20is%20given%20to,linked)%20in%20various%20bonding%20modes. (accessed 14 March 2024).

83 Luo H *et al.* 2021 Progress and Perspectives in Photo- and Electrochemical-Oxidation of Biomass for Sustainable Chemicals and Hydrogen Production. Advanced Energy Materials. **11.** See https://onlinelibrary.wiley.com/doi/full/10.1002/aenm.202101180 (accessed 20 February 2024).

84 ReportLinker.com. 2023. Biodiesel in United Kingdom Market, Overview 2023-2027.

85 Luo H *et al.* 2022 Role of Ni in PtNi bimetallic electrocatalysts for hydrogen and value-added chemicals coproduction via glycerol electrooxidation. ACS Catalysis. **12.** 14492-14506. See https://pubs.acs.org/doi/pdf/10.1021/acscatal.2c03907 (accessed 20 February 2024).

An alternative route to glycerol conversion comprises a mix of electrocatalytic and chemical routes, yielding lactic acid – a precursor to a bioderived polymer – with high selectivity above 85%[86]. Whilst the lactic acid market is growing, this is not large in comparison to primary chemical markets.

Lactic acid can be obtained directly via the fermentation of sugars present in biomass[87]. However, recent studies suggest that an electrochemical and chemical route might have both environmental and technoeconomic advantages[88].

Route from biomass to glycerol to lactic acid to end product.

Biodiesel → BYPRODUCT → Glycerol → Lactic acid → Polylactic acid → Consumer product (eg bioplastic cup)
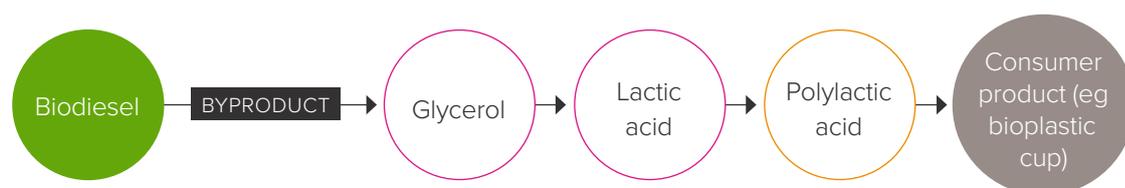
86   Aslam M, Navlani-García M, Cazorla-Amorós D, Luo H. 2023 Efficient and selective glycerol electrolysis for the co-production of lactic acid and hydrogen with multi-component Pt/C-zeolite catalyst. JPhys Materials. **7.** 015002. See https://iopscience.iop.org/article/10.1088/2515-7639/ad0561 (accessed 20 February 2024).

87   Auras R, Loong-Tak L, Selke S, Tsuji H. 2010 Poly(Lactic Acid): Synthesis, structures, properties, processing, and applications. John Wiley & Sons, Inc. See https://onlinelibrary.wiley.com/doi/book/10.1002/9780470649848 (accessed 20 February 2024).

88   Lari G *et al*. 2018 Environmental and economical perspectives of a glycerol biorefinery. Energy Environ. Sci..**11.** 1012. See https://pubs.rsc.org/en/content/articlelanding/2018/ee/c7ee03116e (accessed 20 February 2024).

3.5.2 Co-producing green hydrogen and chemicals from biomass

An advantage of the electrocatalytic processes described above is that these take place in electrolysers, identical to water electrolysis – a well-established technology used in, for example, hydrogen production. Instead of oxidising water to create oxygen at the anode, a bio-derivative is oxidised to produce high value chemicals, such as 5-(hydroxymethyl) furfural (5-HMF) and 2,5-Furandicarboxylic acid (FDCA). At the cathode, green hydrogen is simultaneously produced from the protons contained in biomass – see Figure 7.

Since biomass oxidation takes place at much lower potentials compared to oxidation of water, the total electricity input required is significantly lower, reducing costs for hydrogen production.

The key to realising this technology is developing cost-effective catalysts that can achieve biomass partial oxidation with high activity and high selectivity. The scale of possible hydrogen production is restricted as the hydrogen extraction rate is around 10% of the weight of the total biomass, though it could be used to feed back into the chemical industry at the point of production for further use.

FIGURE 7

Concept of a biomass electrolyser with high value chemicals and green H_2 coproduction.
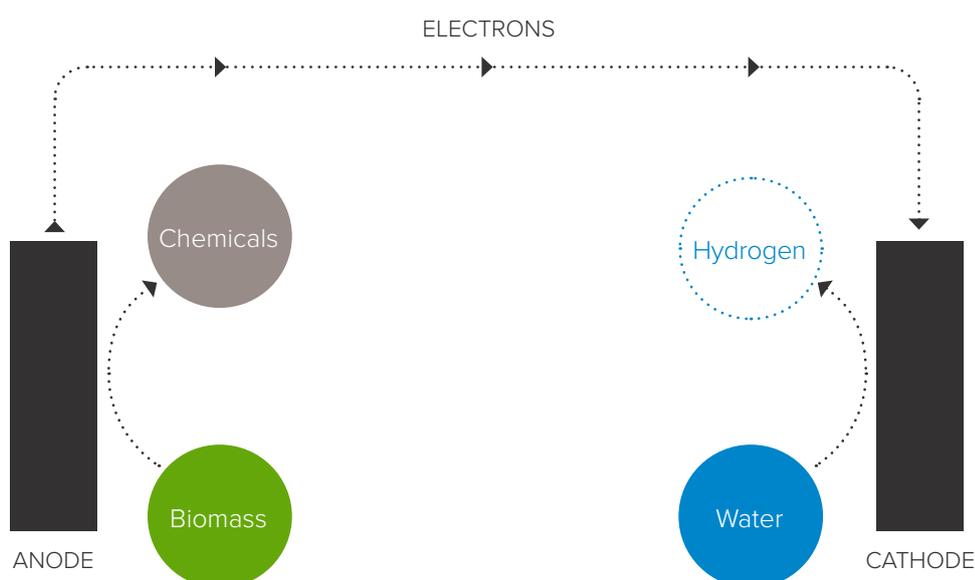
Plastic waste as a feedstock for chemicals

4.1 Types of plastic waste

Plastics are a type of polymer which are composed of thousands to millions of chemically bonded 'monomer' units. These monomers are often either basic chemicals or produced from them. Among the various types of polymers, polyethylene (PE), polypropylene (PP) and polyethylene terephthalate (PET) dominate global plastic waste streams. PE is produced from ethene, PP is produced from propene, and PET is produced from ethene and p-Xylene.

4.2 Plastic waste to chemicals processes

Plastic waste needs to be separated from the wider waste stream for recycling. Mechanical recycling applies forces or heat to reprocess the polymer 'back-to-polymer' into a new product. Chemical recycling applies biochemical processes to chemically breakdown the plastic, potentially back into monomers, in which case it can also be known as 'back-to-monomer' recycling. Chemical recycling differs from mechanical recycling in that it creates a feedstock for chemical production.

4.2.1 Mechanical recycling

Mechanical recycling breaks waste plastics down into flakes or pellets through physical processes including shredding, pressing and melting[89]. Mechanical recycling can be energy efficient, avoiding the need to break down to primary chemicals. However, not all products can be mechanically recycled. There are also limits to mechanical recycling, such as compromised product performance, as well as the introduction of virgin product and additives, which can raise sustainability concerns.

Purification can allow for the whole polymer to be recovered without additives and impurities, using a solution to separate the polymer chains[90]. This could be thought of as a variant of 'back-to-polymer' recycling method. The main products undergoing purification are PE, PP, PVC and polystyrene[91]. However, solvent-based purification recycling is not operating at any meaningful scale. The recycling rates of PP and polystyrene are very low and PVC is hardly recycled at all.

4.2.2 Chemical recycling

Chemical recycling converts waste plastic into monomers, other hydrocarbons or chemicals[92]. There are numerous types of chemical recycling technologies and processes, which are suited to different polymer types and are at different stages of maturity[93].

89 Royal Society of Chemistry. Mechanical recycling. See https://www.rsc.org/globalassets/22-new-perspectives/sustainability/progressive-plastics/explainers/rsc-explainer-5---mechanical-recycling.pdf (accessed 20 February 2024).

90 WRAP. 2023 Plastic recycling reimagined: A high-level overview of non-mechanical recycling. See https://wrap.org.uk/sites/default/files/2023-10/Plastic%20Recycling%20Reimagined%20-%20Overview%20of%20Non-mechanical%20Recycling%20%28003%29.pdf (accessed 20 February 2024).

91 British Plastics Federation. Chemical recycling 101. See https://www.bpf.co.uk/plastipedia/chemical-recycling-101.aspx (accessed 20 February 2024).

92 UN Environment Programme. 2023 Turning off the tap: How the world can end plastic pollution and create a circular economy. See https://wedocs.unep.org/bitstream/handle/20.500.11822/42277/Plastic_pollution.pdf?sequence=3 (accessed 20 February 2024).

93 WRAP. *Op. cit.*

It is possible to use heat or catalytic reactions to convert waste plastics into simple monomers, oils and gases[94]. This can be done via hydrothermal treatment or gasification into syngas, pyrolysis, and enzymatic polymer recycling[95,96]. This can be a challenging process for some polymer types, such as polyethylene or polypropylene, since it requires very high temperatures and is unselective, meaning it does not cleanly yield back the monomer, such as ethene or propene.

The chemistry of other chemical recycling routes depends on the polymer under consideration. For polyesters, such as PET and polylactic acid (PLA), it involves processes such as solvolysis, hydrolysis, alcoholysis or glycolysis. These reactions occur under accessible temperatures and are selective for monomer production. However, these reactions will not work with PE, PP, polystyrene or other commodity hydrocarbon plastics[97].

4.3 Plastic waste availability

Approximately 300 – 400 Mt of plastic is produced annually[98,99]. This range is an indication of varying standards and types of reporting, such as whether textiles are included, and difficulties with verification. Plastic production has rapidly increased in recent decades and will continue to do so for the next several decades under a business-as-usual scenario[100], potentially reaching 1 Gt by 2050[101,102]. As there are a wide range of uses for polymers, there are also many sources of waste for potential to use as a feedstock, including clothing, plastic products, pipes and plastic packaging.

Globally, approximately 9% of all plastic waste is currently recycled[103]. It is important to note that actual recycling rates vary widely between and within countries[104] and there is uncertainty around exact recycling figures and reporting.

94 WRAP. *Op. cit*.

95 Gamerith C *et al*. 2017 Enzymatic recovery of polyester building blocks from polymer blends. Process Biochemistry. **59.** 58-64. See https://www.sciencedirect.com/science/article/abs/pii/S1359511317300090 (accessed 20 February 2024).

96 Benninga J, Jager J, Folkersma R, Voet V, Loos K. 2023 Enzymatic recycling of polyurethanes. In: Cheng H, Gross R. (eds.) Sustainable green chemistry in polymer research. Volume 1. Biocatalysis and biobased materials. American Chemical Society. See https://pubs.acs.org/doi/abs/10.1021/bk-2023-1450.ch005 (accessed 20 February 2024).

97 British Plastics Federation. *Op. cit*.

98 Our World in Data. Plastic pollution. See https://ourworldindata.org/plastic-pollution (accessed 20 February 2024).

99 OECD. Global plastics outlook: Economic drivers, environmental impacts and policy options. See https://www.oecd-ilibrary.org/sites/de747aef-en/index.html?itemId=/content/publication/de747aef-en (accessed 20 February 2024).

100 UN Environment Programme. *Op. cit*.

101 Vidal F *et al*. 2024 Designing a circular carbon and plastics economy for a sustainable future. Nature. **626.** 45-57. See https://www.nature.com/articles/s41586-023-06939-z#:~:text=We%20propose%20a%20circular%20 carbon,use%20and%20recycled%20into%20new (accessed 20 February 2024).

102 Dees J, Sagues W, Woods E, Goldstein H, Simon A, Sanchez D. 2023 Leveraging the bioeconomy for carbon drawdown. Royal Society of Chemistry Green Chem. See https://www.researchgate.net/publication/369870881_ Leveraging_the_bioeconomy_for_carbon_drawdown (accessed 20 February 2024).

103 Hornain J. 2022 Plastics feedstock & pollution: what solutions? World Material Forum. See https://worldmaterialsforum. com/files/Presentations2022/WMF2022-Plastics-Recycling-Jean-Hornain.pdf (accessed 20 February 2024).

104 UN Environment Programme. *Op. cit*.

Without policy intervention, low collection rates may significantly impact the viability of plastic waste as a carbon source for chemical production, particularly in countries with low recovery and recycling rates.

Plastic waste is a well-recognised source of environmental pollution, with approximately 80 Mt of global plastic waste being 'mismanaged'[105] – not stored in secure landfills, recycled or incinerated. Of that, 19 Mt is leaked into the environment, of which 13 Mt enters terrestrial environments, 6 Mt enters rivers and coastlines and 1.7 Mt is then transported to the ocean[106]. Assigning an economic value to this material has the potential create a market and thus reduce plastic waste in the environment. Early-stage research has demonstrated potential for recycling plastic from the marine environment[107].

Improving recycling rates could greatly increase the availability of plastic waste as a feedstock, as well as reduce demand for primary chemical production[108] and virgin fossil feedstock input. This would reduce competition pressure for alternative chemical feedstocks to produce polymers. However, polymer reuse (apart from mechanical recycling) is currently mostly very energy intensive – leading to high associated emissions, if powered by fossil energy.

This is a further challenge to consider when comparing the sustainability or emissions intensity of virgin fossil feedstock-derived products to chemically recycled feedstocks.

To significantly reduce emissions and environmental issues associated with plastic production, whilst providing an alternative source of carbon for chemicals compared to virgin fossil carbon, recycling rates will have to significantly expand – with some estimating a potential required recycling rate of between 70 – 90%[109,110,111]. This is a vast increase on present recycling rates and would require significant policy intervention and system redesign.

105 OECD. *Op. cit.*

106 OECD. *Op. cit.*

107 Ronkay F, Molnar B, Gere D, Czigany T. Plastic waste from marine environment: Demonstration of possible routes for recycling by different manufacturing technologies. Waste Management. **119**. 101-110. See https://www.sciencedirect.com/science/article/pii/S0956053X20305407 (accessed 17 April 2024).

108 Lopez *et al*. *Op. cit.*

109 International Energy Agency. 2018 *Op. cit.*

110 Vidal F *et al*. 2024 Designing a circular carbon and plastics economy for a sustainable future. Nature. **626.** 45-57. See https://www.nature.com/articles/s41586-023-06939-z#:~:text=We%20propose%20a%20circular%20carbon,use%20and%20recycled%20into%20new (accessed 20 February 2024).

111 Bachmann M *et al*. 2023. Towards circular plastics within planetary boundaries. Nature Sustainability. **6.** 599-610. See https://www.nature.com/articles/s41893-022-01054-9 (accessed 14 March 2024).

4.4 Challenges and future research needs

The utilisation of waste plastics for conversion into chemicals is now the focus of intensive research, leading to new ideas about processing routes. However, challenges persist.

In the short to medium term, the plastic waste stream could be a promising feedstock for the substitution of virgin fossil carbon, as it is available in significant quantities. A major challenge to significantly expanding this route is the low rate of waste collection. Over the longer term, there is a fundamental question about the continued growth rate of plastic production. Significantly reducing plastic production could act as a limiting factor on the amount that can be used a feedstock for chemicals but would ultimately also reduce demand on total feedstock requirements – whilst having further benefits for emissions and the environment.

Alongside collection and waste management challenges, there are further pressing research needs to improve the viability of plastic waste as a chemical feedstock.

Chemical recycling is already commercially feasible using PET but is much less well established for other materials[112]. Further understanding of the non-mechanical recycling mechanisms, development of catalysts and processes, and assessment of yield, energy consumption and sustainability are needed to evaluate the material and energy efficiency in comparison to the current production of virgin plastics using fossil fuels. An increasing uptake of chemical recycling would require investment into a greater level of waste separation, advanced chemical recycling infrastructure, and asset modification[113].

Gasification to syngas offers the possibility of building longer chain molecules via methanol synthesis and then methanol-to-olefins or Fischer-Tropsch to straight chain hydrocarbons via syngas[114]. Improving and optimising the selectivity of the process presents an opportunity for further research.

There may be routes that do not require waste type separation, which is one of the main challenges with waste management. Liquefaction of solid wastes containing both biogenic and recycled carbon, is currently being scaled up via demonstration units worldwide[115], but further research is needed to optimise the process at the commercial scale.

The advantage of this approach is that it could potentially integrate with existing steam crackers and downstream facilities. Olefins, the backbone of much of the chemicals industry, are produced directly from fractions of the pyrolysis liquid without passing through an intermediate, such as methanol. A disadvantage is the formation of lighter and heavier fractions, which need reprocessing. Catalytic pyrolysis is being explored as a way of increasing the selectivity of the process[116]. However, it is not yet commercially possible to use pyrolysis oil in steam crackers at any significant scale, as the amount of plastic pyrolysis oil that can be fed into a steam cracker is less than 10%.

112 British Plastics Federation. Chemical recycling 101. See https://www.bpf.co.uk/plastipedia/chemical-recycling-101.aspx (accessed 20 February 2024).

113 Vidal *et al*. *Op. cit*.

114 Nesterenko N *et al*. 2023 Methane-to-chemicals: a pathway to decarbonization. National Science Review. **10.** See https://academic.oup.com/nsr/article/10/9/nwad116/7143128 (accessed 20 February 2024).

115 Plastic Energy. See https://plasticenergy.com/technology/ (accessed 20 February 2024).

116 Miandad R *et al*. 2019 Catalytic pyrolysis of plastic waste: Moving toward pyrolysis based biorefineries. Front. Energy Res. **7.** See https://www.frontiersin.org/articles/10.3389/fenrg.2019.00027/full (accessed 20 February 2024).

CO_2 as a feedstock for chemicals

5.1 Sources of CO_2

Point sources of CO_2 and direct air capture (DAC) of atmospheric CO_2 are the two main potential sources of CO_2 that could be used as a feedstock for chemicals. These are both a form of carbon capture and utilisation (CCU)[117].

5.1.1 Point sources of CO_2

Point sources of CO_2 are typically found at large industrial facilities that emit waste CO_2. Examples include power stations, cement and steel factories, chemical manufacturing like ammonia production, paper and waste incinerators, and brewing or bioethanol production plants. The precise ratio of CO_2 in these emissions varies. For example, cement emissions comprise 75 – 90% CO_2 [118], whilst natural gas power stations emissions are just 4 – 5% [119].

The purity of the CO_2 is important for any subsequent chemical production. Coupling these processes with capture provides an opportunity both to concentrate and purify the waste gas emissions. Specifications for CO_2 purity are helpful for understanding the potential to integrate with chemical manufacturing [120,121]. The typical 'pipeline' specifications are set to >95% CO_2 with parts per million level limitations on the quantity of water, oxygen, carbon monoxide, sulphur and nitrogen oxide contaminants. There is a slightly higher (a few percent) level tolerance of nitrogen (N_2), argon and methane as impurities. These specifications are likely to be quite well aligned with some chemical processes but may present challenges in others, most obviously catalyst poisoning in electrochemical processes.

5.1.2 Direct air capture (DAC) of CO_2

DAC differs from point source CCU in that the technology removes CO_2 directly from the atmosphere, rather than from a specific source. There is clearly a very significant difference in CO_2 concentration between the two, with DAC needing to capture and concentrate starting from 0.04% CO_2. The highly dilute CO_2 in the air means that any uses in chemical manufacturing will require a very significant energy input both to capture and concentrate it.

There are two main types of DAC technology being explored: solid DAC, using adsorbents, where capture occurs at relatively low pressures and medium temperatures, and liquid DAC, which uses a solution and high temperatures to extract CO_2 [122]. DAC is currently a nascent technology, which appears to be viable in countries with specific geologies and readily available renewable energy. Because it is so energy intensive to concentrate atmospheric levels of CO_2, DAC would require a vast supply of energy. To limit emissions associated with this energy and

117 Galimova T *et al*. Global demand analysis for carbon dioxide as raw material from key industrial sources and direct air capture to produce renewable electricity-based fuels and chemicals. Journal of cleaner production. **373.** 133920. See https://www.sciencedirect.com/science/article/pii/S0959652622034928 (accessed 20 February 2024).

118 Meunier N, Laribi S, Dubois L, Thomas D, De Weireld G. 2014 CO_2 capture in cement production and re-use: first step for the optimization of the overall process. Energy Procedia. **63.** 6492-6503. See https://www.sciencedirect.com/science/article/pii/S1876610214025004?ref=pdf_download&fr=RR-2&rr=84e0cbb51807dd80 (accessed 20 February 2024).

119 National Energy Technology Centre. Point source carbon capture from power generation sources. See https://netl.doe.gov/carbon-capture/power-generation#:~:text=Although%20flue%20gases%20from%20NGCC,compression%20in%20an%20NGCC%20plant. (accessed 20 February 2024).

120 Race J, Wetenhall B, Seevam P, Downie J. 2021 Towards a CO_2 pipeline specification: defining tolerance limits for impurities. The Journal of Pipeline Engineering. **11.** 173-190. See https://strathprints.strath.ac.uk/51714/ (accessed 20 February 2024).

121 European Industrial Gases Association. 2016 Carbon dioxide food and beverages grade, source qualification, quality standards and verification. See https://www.eiga.eu/uploads/documents/DOC070.pdf (accessed 20 February 2024).

122 International Energy Agency. Direct air capture. See https://www.iea.org/energy-system/carbon-capture-utilisation-and-storage/direct-air-capture (accessed 20 February 2024).

Image:
A petrochemical plant, a potential point source of carbon from waste CO_2 emissions. © iStock.com / Aliaksandr Yarmashchuk.

DAC as a process, this energy supply would have to be sourced from renewable energy. There will also be cross-sectoral competition for that energy, which could act as a limiting factor on the viability of DAC.

5.2 CO_2 to chemicals processes

CO_2 is already used to make chemicals including urea (for fertilisers), methanol, carbonates and polymers[123]. The thermodynamic stability of CO_2 means that many transformations require significant energy input[124]. This energy must be low carbon to reduce associated Scope 1 and 2 emissions. Life Cycle Assessments of the thermodynamics and economics will be needed to understand the net contribution of specific uses of CO_2 [125].

The potential chemistries to convert CO_2 into chemicals are almost all catalytic processes and often require both vast energy input and other chemicals to work. There are different ways the energy can be input to these processes, including by heating (thermochemical), electrically or, in the longer-term, by sunlight.

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123 Hepburn C *et al*. 2019 The technological and economic prospects for CO_2 utilization and removal. Nature. **575.** 87-97. See https://www.nature.com/articles/s41586-019-1681-6 (accessed 20 February 2024).

124 Royal Society. 2017 The potential and limitations of using carbon dioxide. See https://royalsociety.org/-/media/policy/projects/carbon-dioxide/policy-briefing-potential-and-limitations-of-using-carbon-dioxide.pdf (accessed 20 February 2024).

125 *Ibid*.

The most technologically advanced catalytic routes for the conversion of CO_2 include methanation to produce methane, direct methanol synthesis and other alcohols, and syngas production using the water-gas shift reaction followed by methanol synthesis or Fisher-Tropsch to produce hydrocarbons. All these processes require a large amount of hydrogen and heat. However, these technologies require further development to be commercially viable.

Electrocatalysis converts CO_2 into a variety of products in an electrochemical cell through the application of an electrical voltage. The main challenges of the current technologies are: maintaining selectivity to the desired carbon-based product; the very low solubility of CO_2 in water; the need for extra voltage to drive the reactions, which leads to energy inefficiencies; and intolerance to feed impurities. One of the main advantages is that electrocatalytic CO_2 conversion can be integrated with renewable energy sources: without doing so, the technology would cause a net increase in emissions[126] and be counterproductive to any efforts to transition the chemical sector to help meet net zero targets.

Carbon monoxide can be made by the reaction of CO_2 with hydrogen that can be produced from water. This is the high temperature shift reaction, which is a well-known process. A potential alternative to this shift reaction is thermochemical cycling, which provides an opportunity to split water and reduce CO_2 into syngas using reduction-oxidation (redox) cycles. This technology has high theoretical efficiencies. However, it currently suffers from low efficiencies due to the large temperature swing between redox steps. Isothermal or near-isothermal operation with implementation has been demonstrated by pressure-swing, enhancing heat efficiency and fuel yield[127]. Further research should be directed towards high temperature energy storage, solid-solid heat recuperation, and oxygen separation for achieving high solar-to-fuel conversion efficiencies.

At the very early research stage, photoelectrochemical routes can potentially convert CO_2 into syngas by combining light and electrochemical driven steps, whilst other studies have explored novel photoelectrochemical routes that combine CO_2 conversion with plastic-to-chemical conversion[128]. However, all these routes are at very early stages of development and are a long way off being realisable. This field of research remains at an academic discovery stage and there are still fundamental challenges to be overcome.

126 Kauffman D *et al*. 2015 Efficient electrochemical CO_2 conversion powered by renewable energy. ACS Appl. Mater. Interfaces. **7.** 15626-15632. See https://pubs.acs.org/doi/abs/10.1021/acsami.5b04393 (accessed 20 February 2024).

127 Tran J *et al*. 2023 Pressure-enhanced performance of metal oxides for thermochemical water and carbon dioxide splitting. Joule. **7.** 1759-1768. See https://www.sciencedirect.com/science/article/abs/pii/S2542435123003148 (accessed 20 February 2024).

128 Bhattacharjee S *et al*. 2023 Photoelectrochemical CO_2-to-fuel conversion with simultaneous plastic reforming. Nature Synthesis. **2.** 182-192. See https://www.nature.com/articles/s44160-022-00196-0 (accessed 20 February 2024).

Another option to use CO_2 is to produce carbonates and polymers by combining it with other chemicals[129]. This utilisation does not rely on any hydrogen or reductant and can be economically attractive since the CO_2 replaces petrochemicals. For example, CO_2 copolymerisation with epoxides produces polycarbonate polyols used to make insulation foams, coatings, sealants, adhesives and elastomers[130,131]. This technology is therefore advanced as a CO_2 utilisation. CO_2 can also be reacted with epoxides to produce cyclic carbonates, essential electrolytes for batteries and electric vehicles[132]. These uses of CO_2 are covered in a previous Royal Society report on the potential and limitations of using carbon dioxide[133].

5.3 Availability of CO_2

There is currently a high potential availability of CO_2 from point sources, due to the number of large industrial and power plants using fossil fuels or bioethanol. Industrial point sources could meet demand for chemical sector CO_2 use in 2030 but would likely not suffice by 2050[134], as point sources of CO_2 decline in the context of net zero ambitions and demand across other sectors increases. It is further necessary to consider how the choice of CO_2 source affects the climate impact, eliminating some sources for select product categories[135].

To meet the growing demand for CO_2, DAC supply would have to expand significantly. At present, DAC plants capture approximately 0.01 Mt CO_2 per year[136]. Plants under construction or in advanced development will likely only be able to capture around 4.7 Mt CO_2 per year by the end of this decade. Under the International Energy Agency's Net Zero by 2050 scenario, DAC expands to just under 1 Gt CO_2 by 2050[137].

129 Hepburn *et al. Op. cit.*

130 Deacy A, Phanopoulos A, Lindeboom W, Buchard A, Williams C. 2022 Insights into the mechanism of carbon dioxide and propylene oxide ring-opening copolymerization using a Co(III)/K(I) heterodinuclear catalyst. J. Am. Chem. Soc. **144.** 17929-17938. See https://pubs.acs.org/doi/full/10.1021/jacs.2c06921 (accessed 14 March 2024).

131 Hepburn *et al. Op. cit.*

132 *Ibid.*

133 Royal Society. 2017 The potential and limitations of using carbon dioxide. See https://royalsociety.org/-/media/policy/projects/carbon-dioxide/policy-briefing-potential-and-limitations-of-using-carbon-dioxide.pdf (accessed 14 March 2024).

134 Lopez *et al. Op. cit.*

135 Mason F, Stokes G, Fancy S, Sick F. 2023 Implications of the downstream handling of captured CO_2. Front. Clim. **5.** See https://www.frontiersin.org/articles/10.3389/fclim.2023.1286588/full (accessed 18 March 2024).

136 International Energy Agency. Direct air capture. *Op. cit.*

137 International Energy Agency. 2021 Net zero by 2050: A roadmap for the global energy sector. See https://iea.blob.core.windows.net/assets/deebef5d-0c34-4539-9d0c-10b13d840027/NetZeroby2050-ARoadmapfortheGlobalEnergySector_CORR.pdf (accessed 20 February 2024).

At present, approximately 0.2 Gt of CO_2 is used globally each year[138], of which around half is used to produce urea fertiliser and around a third is used for the extraction of crude oil through enhanced oil recovery[139]. To achieve a significant scale up of CCU, there would have to be developments in both capture and utilisation technologies, access to sufficient low-cost renewable energy and other resources such as water, and changes in the policy and funding landscape[140]. DAC currently costs around USD $200 – 600 per tonne of CO_2 removed[141]. This would have to fall to make large scale chemical production from DAC CO_2 competitive.

There will also be competing demands for CO_2 in other sectors, such as for concrete and building materials. There is also growing interest in the use of DAC CO_2 for synthetic fuels for transportation, for heating and, to a less extent, in the power sector[142,143].

There are various future estimates of how much CO_2 the chemicals sector could utilise, given this competing demand. Lower end estimates suggest 0.2 – 0.6 Gt CO_2 could be used to produce polymers and other chemical products[144,145,146]. Higher end estimates propose that the chemical industry may require as much as between 2.8 Gt[147] up to 4.7 Gt in 2050[148].

It is difficult to estimate exact supply and demand, given the infancy of some technological routes, overcoming the energy requirements to turn CO_2 into reduced carbon molecules and the changing policy landscape.

It is also important to note that the estimates of the overall scale of CO_2 utilisation for chemicals is less than 1%[149] of annual anthropogenic input of CO_2 into the atmosphere (~59 Gt CO_2 equivalent[150]).

138 International Energy Agency. 2019 Putting CO_2 to use. See https://iea.blob.core.windows.net/assets/50652405-26db-4c41-82dc-c23657893059/Putting_CO2_to_Use.pdf (accessed 20 February 2024).

139 *Ibid*.

140 Dhakal *et al. Op. cit.*

141 World Resources Institute. 6 things to know about direct air capture. See https://www.wri.org/insights/direct-air-capture-resource-considerations-and-costs-carbon-removal (accessed 20 February 2024).

142 National Academies. Carbon dioxide utilization markets and infrastructure. See https://nap.nationalacademies.org/catalog/26703/carbon-dioxide-utilization-markets-and-infrastructure-status-and-opportunities-a (accessed 18 March 2024).

143 Sick V *et al*. 2022 Implementing CO_2 capture and utilization at scale and speed. Global CO2 Initiative. See https://deepblue.lib.umich.edu/handle/2027.42/174094 (accessed 18 March 2024).

144 Royal Society. 2017 *Op. cit.*

145 Olfe-Krautlein B, Naims H, Bruhn T, Lafunete A, Tobias M. 2014 IASS Fact Sheet 2/2014: carbon dioxide as an asset? Potsdam: IASS (Institute for Advanced Sustainability Studies). See https://publications.rifs-potsdam.de/rest/items/item_2793988_6/component/file_2793989/content (accessed 20 February 2024).

146 Otto A, Grube T, Schiebahn S, Stolten D. 2015 Closing the loop: captured CO2 as feedstock in the chemical industry. Energy. Environ. Sci. **8.** 3283-3284. See https://pubs.rsc.org/en/content/articlelanding/2015/ee/c5ee02591e (accessed 20 February 2024).

147 Galimova T *et al*. Global demand analysis for carbon dioxide as raw material from key industrial sources and direct air capture to produce renewable electricity-based fuels and chemicals. Journal of Cleaner Production. **373.** 133920. See https://www.sciencedirect.com/science/article/pii/S0959652622034928 (accessed 20 February 2024).

148 Lopez *et al. Op. cit.*

149 Mac Dowell N, Fennell P, Shah N, Maitland G. 2017 The role of CO_2 capture and utilization in mitigating climate change. Nature Climate Change. **7.** 243-249. See https://www.nature.com/articles/nclimate3231 (accessed 18 March 2024).

150 Intergovernmental Panel on Climate Change. 2022 Climate Change 2022 Mitigation of climate change: Summary for policymakers. See https://www.ipcc.ch/report/ar6/wg3/downloads/report/IPCC_AR6_WGIII_SPM.pdf (accessed 18 March 2024).

5.4 Future challenges of CO_2 to chemicals

As discussed, the production of chemicals from CO_2 is feasible at a limited scale but requires enormous quantities of green hydrogen and renewable power[151]. The production of ethene and other hydrocarbons needs more development, including in catalysis, means of driving processes (heat or electricity), process and reactor design and coupling with other chemical manufacturing. For thermochemical catalysis, the focus has been on reducing the temperature for the reduction pathways, driving selectivity higher and improving tolerance to water, which is a common by-product of these reductions[152].

There is a major effort to transform CO_2 into higher alcohols directly, avoiding the need for methanol as an intermediary. Such chemistry could be advantageous as a direct route to high-value surfactants, lubricants and intermediates in the chemical industry[153].

The copolymerisation of CO_2 with other monomers continues to focus on diversifying the range of polymers produced, increasing catalytic activity and selectivity, and designing processes that are accelerated by common impurities, such as water[154].

More generally, catalytic chemistry that functions using mixtures or inhomogeneous supplies of raw materials, including CO_2, is an active research field[155]. Carboxylation chemistry also provides routes, independent of hydrogen, to produce carboxylic acids, esters and carbonates which are useful as both monomers but also products in their own right[156].

Electrocatalysis offers another interesting opportunity to create products from CO_2, with a significant research effort into ethene, ethanol and propanol production[157].

151 Artz J *et al*. 2018 Sustainable conversion of carbon dioxide: An integrated review of catalysis and life cycle assessment. Chem. Rev. **118.** 434-504. See https://pubs.acs.org/doi/10.1021/acs.chemrev.7b00435 (accessed 20 February 2024).

152 *Ibid*.

153 Huang J *et al*. 2023 The synthesis of higher alcohols from CO_2 hydrogenation over Mn-Cu-K modified Fe5C2 and CuZnAlZr tandem catalysts. Energy Res. **10.** See https://www.frontiersin.org/articles/10.3389/fenrg.2022.995800/full (accessed 20 February 2024).

154 Plajer A, Williams C. 2022 Heterocycle/Heteroallene ring-opening copolymerization: Selective catalysis delivering alternating copolymers. Angew. Chem. Int. Ed. **61.** See https://onlinelibrary.wiley.com/doi/epdf/10.1002/anie.202104495 (accessed 20 February 2024).

155 Deacy *et al. Op. cit.*

156 Artz *et al. Op. cit.*

157 Li F *et al*. Molecular tuning of CO_2-to-ethylene conversion. Nature. **577.** 509-513. See https://www.nature.com/articles/s41586-019-1782-2 (accessed 20 February 2024).

These processes typically depend on copper catalysts. There is on-going research focusing on innovative reactors, flow engineering, improving carbon mass balance, improving catalyst lifetime and tolerance to impurities, as well as integrating the reductive chemistry with other chemical oxidations.

Photochemical and photoelectrochemical CO_2 conversions are at a much earlier technical stage, with research needed to identify the most promising photoactive materials, catalysts and to prevent decay processes[158]. The production of prototype devices and engineering of the materials interfaces is also an important current and future research field.

Further research is required to lower the energy requirements and improve the efficiency of DAC technologies, as well as around diversifying and scaling the range of products possible from CO_2. For example, there is significant potential to use CO_2 in polymers to toughen structures and make them more resilient[159]. Further research and investment could focus on the conversion of CO_2 to syngas for onward conversion to fuels and intermediate chemicals[160], the conversion of CO_2 to oxygenated chemicals, and the reduction of CO_2 to alcohols.

5.5 Emerging routes from CO_2 to chemicals

The role of green methanol as a building block might become more prominent in a transition away from fossil feedstocks. Green methanol can be produced via thermal CO_2 conversion using green hydrogen, which is a well-established route. Green methanol could also potentially be produced from the bio-chemical transformation of biomass, though these technologies are not yet at commercial readiness level[161].

New chemical transformations, such as the recently developed methanol-to-olefins and methanol-to-aromatics processes, are alternate ways of producing olefins and aromatics[162]. It is important to note that these technologies have been developed in the context of using coal-based methanol as input[163], which results in higher overall emissions than using naphtha or natural gas as feedstocks, but emissions would be lower if using green methanol. Further work is required to enhance the technology to commercialisation standard.

158 Moore E, Andrei V, Oliveira A, Coito A, Pereira I, Reisner E. 2021 A semi-artificial photoelectrochemical tandem leaf with a CO_2-to-formate efficiency approaching 1%. Angew. Chem. Int. Ed. **60.** 26303-26307. See https://onlinelibrary.wiley.com/doi/10.1002/anie.202110867 (accessed 20 February 2024).

159 Sulley G *et al*. 2020 Switchable catalysis improves the properties of CO_2-derived polymers: poly(cyclohexene carbonate-b-ε-decalactone-b-cyclohexene carbonate) adhesives, elastomers, and toughened plastics. J. Am. Chem. Soc. **142.** 4367-4378. See https://pubs.acs.org/doi/full/10.1021/jacs.9b13106 (accessed 20 February 2024).

160 Lu S, Shi Y, Meng N, Lu S, Yu Y, Zhang B. 2020 Electrosynthesis of syngas via the co-reduction of CO_2 and H_2O. Cell Reports Physical Science. **1.** See https://www.cell.com/cell-reports-physical-science/pdf/S2666-3864(20)30255-1.pdf

161 International Renewable Energy Agency. *Op. cit*.

162 Dechema. 2017 Low carbon energy and feedstock for the European chemical industry. See https://dechema.de/dechema_media/Downloads/Positionspapiere/Technology_study_Low_carbon_energy_and_feedstock_for_the_European_chemical_industry.pdf

163 Lopez *Op. cit*.

Further considerations for alternative feedstocks

6.1 Future feedstock mix of the chemical industry

While exploratory estimates of the potential future mix of each of the alternative carbon sources and fossil feedstocks do exist, it is important to note that it is not possible to predict the exact future mix of chemical feedstocks. This will change over time as technologies develop, countries make policy and regulatory changes, and individual businesses make varying investment decisions. The mix of chemical feedstocks will also change between places for similar reasons, as well as the differing geographies and availabilities of feedstocks between countries.

To replace all fossil carbon in chemicals, it is likely that a combination of biomass, waste and CO_2 sources will be required[164] – and that this mix will vary over time. Whilst this may help to reduce supply chain risks through diversification, and potentially help reduce sustainability risks of overconsuming one particular feedstock type, it will introduce far greater heterogeneity into the chemical industry supply chain than exists today.

However, there is also an opportunity to use alternative carbon sources to bypass the existing primary chemicals stage straight to downstream, higher value or speciality chemicals. Advances in industrial biotechnology might open the door to bio-manufacturing routes of alternative chemical 'building-blocks' such as acetone, alcohols such as butanol and isopropanol (in addition to methanol) or directly to high value chemicals from biomass, plastics and CO_2[165,166]. As discussed, biomass routes are difficult to scale to commodity levels and may be more effective at more limited scales for speciality chemicals – which subsequently impacts the emissions reductions potential.

Transitioning away from fossil feedstocks may require some businesses to operate in a less centralised structure with more modularity[167], as distributed feedstocks and energy requires a distributed approach to manufacturing. Whilst this is not in the scope of this report and requires further investigation, challenges include a loss of economy of scale and heat integration, with subsequent impacts on cost and energy efficiency.

164   S&P Global. Decarbonizing chemicals part one: Sectorwide challenges will intensify beyond 2030. See https://www.spglobal.com/esg/insights/featured/special-editorial/decarbonizing-chemicals-part-one-sectorwide-challenges-will-intensify-beyond-2030 (accessed 20 February 2024).

165   International Energy Agency. 2020 Bio-based chemicals. See https://www.ieabioenergy.com/wp-content/uploads/2020/02/Bio-based-chemicals-a-2020-update-final-200213.pdf (accessed 20 February 2024).

166   Li F *et al*. 2019 Cooperative CO_2-to-ethanol conversion via enriched intermediates at molecule–metal catalyst interfaces. Nature Catalysis. **3.** 75-82. See https://www.nature.com/articles/s41929-019-0383-7 (accessed 20 February 2024).

167   Tickner J, Geiser K, Baima S 2022 Transitioning the chemical industry: Elements of a roadmap toward sustainable chemicals and materials. Environment: science and policy for sustainable development. **64.** 22-36. See https://journals.scholarsportal.info/details/00139157/v64i0002/22_ttcieortscam.xml (accessed 20 February 2024).

6.2 Wider sustainability considerations and Life Cycle Assessment

It is critical that any alternative carbon sources for chemicals are assessed for their sustainability, to ensure that they do not have unintended or additional impacts on the environment and society. To classify a carbon source as 'green' and ensure that greenhouse gas emissions are not reduced at the expense of other impacts, issues such as resource depletion, acidification, eco- and human toxicity, land use, biodiversity and energy requirements should all be evaluated. The energy requirements and initial source of carbon for all alternative feedstocks must be critically assessed to ensure that both climatic and wider environmental implications are not worsened. Accounting for claims of 'carbon neutrality' or 'net negative emissions' need to be considered and documented carefully, to avoid risks of greenwashing or overstating the benefits of one feedstock type over another.

Addressing further social impacts, such as on food security, are also critical to ensure that any transition away from fossil feedstocks in chemicals does not have wider implications on society.

Life Cycle Assessment (LCA) is one approach that can be used to assess the impacts of the acquisition, processing, transport, use stage and end-of life of different feedstocks. However, comparability between LCA studies is often difficult, due to varying assumptions and system boundaries used. Further research in this area to better understand the life cycle and sustainability of different carbon sources could subsequently inform policymaking and help improve standardisation across industry.

6.3 Investment and growth opportunities

There are significant opportunities for individual companies and national governments to act as early innovators and leaders in the transition to alternative carbon sources. A drive for developing novel processes and technologies could offer opportunities for large-scale investment into chemistry research and development, innovation, and skills training. The chemical industry is already a major source of research and innovation investment in some countries, such as the UK[168] – see Box 6. This could be accelerated further as new processes and technologies are required for the future chemical industry.

Transitioning away from fossil feedstocks to alternative carbon sources does present challenges to the chemical sector, which has co-developed alongside the fossil fuel industry over the last century. A long-term, cross-sectoral, stable policy landscape could help to address these risks and mitigate against existing challenges some regions face around job losses and offshoring[169].

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BOX 6

Opportunities for the UK

There are approximately 4,500 companies in the UK chemical sector, directly employing approximately 150,000 people and supporting a further ~350,000 jobs in the wider supply chain[170]. The sector accounts for 17.5% of total UK business research and development spending, and exports over £50 billion of goods[171].

Whilst the UK chemical industry is highly diverse and geographically spread, there are particular industrial clusters in the North West, North East, Yorkshire and the Humber, and Scotland. Chemical production is currently closely geographically tied to the location of primarily fossil feedstocks and the ethene pipeline and ports in the north of England and in Scotland, whilst speciality chemicals, downstream products, and the wider research base are more geographically diverse.

The UK has a strong chemistry research base through academic institutions, dedicated research facilities and industrial research, with strong collaboration between sectors and disciplines[172].

Across these sectors, there are more than 50,000 people working in scientific research and development[173], whilst the number of chemistry staff and PhD students in academia has increased in recent years[174].

For example, one particular national strength is catalysis science[175], featuring a strong skill base and an increasing number of related small-to-medium enterprises (SMEs)[176]. As discussed, catalysis is central to many of the routes from biomass, plastic waste and CO_2 to chemicals.

More broadly, the UK has international strengths in synthetic organic chemistry[177]. There is an opportunity to support and expand this skill base to meet the high demand from the UK's varied chemical producer and user sector. Through its research base, there is an opportunity for the UK to take a leading role in the research and development of novel science to more sustainable chemicals.

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Conclusion

To reduce emissions and help progress towards net zero, the chemical industry will have to address its Scope 3 emissions by transitioning away from fossil feedstocks to alternative carbon sources. The sector will also have to address Scope 1 and 2 emissions through measures such as energy efficiency and process electrification using renewable energy.

Potential alternative carbon sources include biomass, plastic waste and CO_2. There are both opportunities and challenges associated with each of these feedstock types – see Table 1.

There are already some commercially available routes from biomass to chemicals and polymers: approximately 8% of chemicals are currently produced using biomass feedstocks. There is a growing research base in this area, opening up potential routes to downstream chemicals that bypass existing primary chemicals. However, the viability of biomass to replace all fossil feedstocks is constrained by competing demands, such as for food and aviation fuels, and challenging due to wider sustainability implications on land use and biodiversity. There are also significant technical challenges, particularly regarding processing lignocellulose.

TABLE 1

Summary of alternative carbon sources opportunities and challenges

	OPPORTUNITIES	CHALLENGES
Biomass	Some established routes to chemicals and an extensive research base leading to novel routes Potential to bypass primary chemicals to downstream chemicals	Separation and conversion of lignocellulose Competing cross-sectoral demands Potential wider sustainability concerns
Plastic waste	High potential availability of waste plastics Established route for chemical recycling of PET plastics	Low collection and recovery rates Low technology readiness of chemical recycling routes for non-PET plastics High energy requirements
CO_2	High potential availability from point sources (short- to medium-term) and the atmosphere (long-term)	Low technology readiness and high cost of direct air capture Competing cross-sectoral demands Vast green hydrogen and renewable energy requirements

Plastic waste is another viable route to chemicals and polymers. Mechanical recycling and some chemical recycling routes are already commercially available. Further development of chemical recycling technologies would help scale 'back-to-monomer' recycling, avoiding the issues of impurities, additives and performance decline of mechanically recycled products. Vast scale up of plastic waste recovery and both mechanical and chemical recycling is required to reduce emissions, address pollution and waste mismanagement issues, and reduce demand for virgin fossil carbon. This is particularly important given the forecast rise in plastic production between now and 2050.

Point-source and DAC carbon capture and utilisation is a further alternative source of carbon for chemicals. There is significant potential availability from both point sources and atmospheric carbon. However, the number of point sources of CO_2 will decline over time as industries decarbonise. DAC is currently prohibitively expensive and has vast energy requirements. Both CCU routes to chemicals will require a significant expansion of renewable energy and green hydrogen, to avoid adding further emissions. It is important to recognise that there will also be competition for CO_2, renewable energy and hydrogen across sectors.

To manage the availability, benefits and limitations of all three alternative carbon sources, the future chemical industry will likely have to use a mixture of biomass, plastic waste and CO_2 feedstocks for chemicals manufacture — and a declining proportion of fossil feedstocks over time during the transition. There is no single targeted or desired mix of biomass, plastic waste, or CO_2 feedstocks. This will change over time, as technologies develop,

and between locations as different countries have varying availabilities of each feedstock and different chemical industry characteristics. However, it is important to recognise that the chemical industry will have increasing heterogeneity of feedstock supply in the future, which will require substantial infrastructure and system redesign.

It is critical to assess the emissions and wider sustainability of each alternative feedstock and the various routes from these to chemicals. Whilst each source offers potential to reduce emissions, this will not be realised without sustainable sourcing practices, vastly scaling renewable energy, and addressing products' end-of-life emissions and environmental impacts. Demand reduction can both reduce total chemical sector emissions, whilst potentially supporting the viability of meeting overall demand through alternative carbon feedstocks.

Whilst technologies and routes from each of the proposed alternative feedstocks to chemicals do exist, there will have to be significant further research and development across chemistry and related fields, as well as investment and scale-up to accelerate the transition away from fossil feedstocks and achieve the necessary emissions reductions required. There are potential economic and societal opportunities associated with innovation within many fields of chemistry and chemical engineering.

Long-term, cross-government, international policy coordination could help to support and enable the transition to a net zero chemical industry — capitalising on innovation, investment and growth opportunities, whilst building in resilience of supply to mitigate risks and competing demands.

APPENDIX A

Glossary of terms

Aromatics
Benzene, toluene and mixed xylenes, also known as 'BTX'.

Biomass
Material of biological origin excluding material embedded in geological formations and/or fossilised. Sources include: biomass crops; food crops, such as vegetable oils and starches; agricultural residues; forest residues; horticultural residues; municipal food and garden waste; the biogenic fraction of municipal waste, such as paper and card; and marine biomass.

Carbon capture and storage (CCS)
A process in which a relatively pure stream of CO_2 from industrial and energy-related sources is separated (captured), conditioned, compressed and transported to a storage location for long-term isolation from the atmosphere.

Carbon capture and utilisation (CCU)
A process in which CO_2 is captured and then used to produce a new product. If the CO_2 is stored in a product for a climate-relevant time horizon, this is referred to as CO_2 capture, utilisation and storage (CCUS).

CO_2 equivalent emissions
The amount of CO_2 emissions that would cause the same integrated radiative forcing or temperature change, over a given time horizon, as an emitted amount of a greenhouse gas (GHG) or a mixture of GHGs.

Decarbonisation
Reducing or eliminating CO_2 emissions associated with energy by replacing fossil fuel energy with carbon-free, renewable energy sources.

Defossilisation
Replacing fossil-based carbon feedstocks with non-fossil, renewable carbon sources.

Embedded carbon
Carbon inherent and essential to the molecular structure of chemicals and materials, (usually) not replaceable with non-carbon alternatives.

Ethene
A hydrocarbon with the formula C_2H_4 or $H_2C=CH_2$. It is also commonly known as ethylene. This report uses the International Union of Pure and Applied Chemistry (IUPAC) preferred term 'ethene'.

Feedstock
Unprocessed raw material that can be used to produce chemicals.

Greenhouse gas emissions
The release of greenhouse gases into the atmosphere. Greenhouse gases include CO_2, methane, nitrous oxide and water vapour.

Net zero
Anthropogenic greenhouse gas emissions balanced by anthropogenic removals over a specified period.

Olefins
Ethene, butene and propene.

Petrochemicals
Chemical products derived from
petroleum refining.

Propene
An unsaturated organic compound with the
chemical formula $CH_3CH=CH_2$. Also commonly
known as propylene. This report uses the
International Union of Pure and Applied
Chemistry (IUPAC) preferred term 'propene'.

Primary chemicals
Ethene, propene, butadiene, benzene,
toluene, mixed xylenes and methanol.
Whilst ammonia is usually included in this
grouping, this is not included in this briefing
as it is not a carbon-based chemical and was
the focus of a previous Royal Society report.

Scope 1 emissions
Direct emissions associated with the processes
involved in making the carbon-based chemical.
This includes emissions related to the
combustion of fossil fuels to produce energy
as well as direct process emissions.

Scope 2 emissions
Upstream indirect emissions associated
with purchased electricity for chemical
conversion processes.

Scope 3 emissions
Indirect emissions associated with upstream
and downstream processes. Upstream
processes include the extraction and
production of feedstocks. Downstream
processes include product use and end-of-life
disposal, such as degradation and incineration.

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