



## Defossilising chemical industries

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Chemical industries underpin modern life, producing fuels, polymers, fertilisers, surfactants, solvents, and countless other products. Yet over 90% of feedstocks for carbon-based chemicals come from oil, gas, and coal,<sup>1,2</sup> making the sector the largest industrial consumer of non-energy fossil carbon raw materials, while the chemical industry as a whole is responsible for ~6% of global CO<sub>2</sub>-equivalent emissions.<sup>2-4</sup> Around half of the fossil inputs that are processed by the petrochemical industry are embedded directly into products,<sup>5</sup> locking in fossil carbon for the medium to long-term, but

at the same time driving non-circular, unsustainable carbon flows. While decarbonising energy use is vital, reducing the amount of embedded fossil carbon and replacing it with renewable carbon also demands a fundamental shift in how chemicals are sourced, produced, and treated at the end of life.

Shifting to sustainable, circular carbon use is now central to global policy, reflected in the EU Chemicals Agency Strategy for Sustainability<sup>6</sup> and net-zero roadmaps from the IEA,<sup>7</sup> and the UN Sustainable Development Goals on Responsible Consumption (SDG 12) and Climate Action (SDG 13). Yet the diversity of feedstocks, products, and end-of-life pathways in the chemical industry means addressing these challenges demands broad and integrated research efforts.

This themed collection on defossilising chemical industries brings together original studies, reviews, and perspectives tackling challenges across the sector. Contributions span from the molecular scale through to entire systems, covering microbial and enzymatic routes for valorising carbon-rich waste, to advances in biomass deconstruction, catalytic upgrading, and pathways such as Fischer-Tropsch and conversion of CO<sub>2</sub>. Some papers explore feedstock substitution, product reformulation, and system-level analysis, including process modelling, life cycle assessment (LCA), and techno-economic analysis (TEA). Chemical recycling of existing materials and circularity also feature prominently, with studies examining how carbon can be retained across multiple lifecycles.

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## Biotechnological valorisation of biomass and plastic waste

Biotechnological approaches have unique advantages in terms of selectivity and capacity to carry out multi-step transformations in a single reactor (“one-pot”) while tolerating variable feedstocks, offering promising routes that valorise waste carbon into sustainable carbon-based chemicals. Such routes are illustrated in a perspective article detailing engineered microbial platforms that convert carbon-rich polymeric wastes, including lignocellulose and plastics, into valuable chemicals, moving beyond first-generation biogenic feedstocks to address land-use and associated biodiversity concerns (<https://doi.org/10.1039/D5SU00013K>). An innovative strategy for combining chemical and biotechnological methods for maximising the yield of substrates for fermentation from wood biomass was also presented. In addition to the cellulosic sugars, the lignin stream could be utilised after oxidation, enabling strong growth of five microbial strains (<https://doi.org/10.1039/D5SU00039D>). Another contribution demonstrates the microbial production of polyhydroxyalkanoates (PHAs) from chemically depolymerised lignin. By combining alkaline- and acid-treated lignin streams, the authors show that multiple PHA-producing strains can grow on the resulting neutral mixture and generate biodegradable polyesters, highlighting a potential route to convert low-value lignin into sustainable, bio-based polymers (<https://doi.org/10.1039/D5SU00563A>).

## Chemo- and photocatalytic upgrading of biomass and derivatives

The collection also highlights catalytic upgrading of biomass, a critical route in utilising renewable feedstocks to produce valuable chemicals. One example evaluates routes to furfural production, comparing the industrialised homogeneous sulfuric acid catalysis with

a heterogeneous Amberlyst-70® catalyst and closed-loop process design. This study integrated techno-economic and life cycle assessments to identify key challenges, including catalyst deactivation and lack of by-product valorisation (<https://doi.org/10.1039/D5SU00106D>). Other work probed molecular interactions between lignin-derived compounds and industrial zeolite catalysts, combining vibrational spectroscopy with *ab initio* calculations to map adsorption behaviours across different microporous frameworks. Such insights are essential for adapting conventional catalysts optimised for converting fossil feedstocks to handle biomass feedstocks efficiently (<https://doi.org/10.1039/D5SU00024F>). Further advancing catalyst design, another paper explores the eco-design of ZSM-5 zeolites modified by biomass-derived additives such as lignin and sugarcane bagasse during synthesis. This approach led to more favourable catalyst structures and properties while incorporating agro-industrial waste as a green synthesis agent, demonstrating a scalable route to sustainable catalyst production (<https://doi.org/10.1039/D5SU00072F>). Integrated biorefinery approaches maximising resource efficiency are also showcased, employing marine macroalgae as a less-explored chemical feedstock, employing catalytic oxidation of the carbohydrate component to produce formic acid followed by solvent extraction to enable co-production of a protein-enriched fraction (<https://doi.org/10.1039/D5SU00012B>). Photocatalytic methods are also showcased, with a study into the photoreforming of real industrial biomass-derived wastes using Nb-doped BiVO<sub>4</sub> photoanodes. Niobium incorporation enhances charge transport and catalytic activity, enabling efficient conversion of crude glycerol and flegmass into formic acid and hydrogen under simulated sunlight. This work illustrates a mild, solar-driven route for upgrading complex waste streams while producing low-carbon H<sub>2</sub> (<https://doi.org/10.1039/D5SU00376H>). Together, these studies highlight the potential of innovations in catalyst design and modification in enabling the

chemical sector's transition to a circular, biomass-based industry.

## CO<sub>2</sub> valorisation via Fisher Tropsch synthesis

The use of CO<sub>2</sub> as a carbon feedstock, together with renewable hydrogen or electricity to enable C<sub>1</sub>-based transformations into synthetic fuels is of great importance to circular carbon utilisation. One study explores CO<sub>2</sub> as a co-fed reactant in the transformation of syngas via Fischer-Tropsch-to-olefins (FTO) catalysis, using neutron spectroscopy to reveal hydrogen-rich overlayer species during operation. This provides molecular-scale evidence that CO<sub>2</sub> can influence the chemical environment of Fe-based catalysts, suggesting additional pathways for reactivity control in syngas defossilisation (<https://doi.org/10.1039/D5SU00042D>). In a complementary contribution, manganese distribution within CoMn/TiO<sub>2</sub> catalysts critically affected selectivity of syngas conversion to alcohols and olefins. By comparing synthesis routes that manipulate Mn location (from employing mixed oxides to surface doping) the study shows how tuning local environments can lead to more favourable product profiles and more efficient catalysts for low-carbon fuel production (<https://doi.org/10.1039/D4SU00746H>).

## Economics of biomass valorisation

Understanding whether emerging technologies can deliver real-world impact requires rigorous evaluation of both economic and environmental performance through TEA and LCA analysis. A critical review examines ammonia-based pretreatment of lignocellulosic biomass, highlighting how innovations like Ammonia Fibre Extraction (AFEX) and Compacted Biomass with Recycled Ammonia (COBRA) technologies boost conversion yields, while aligning with circular economy principles through sustainable ammonia production routes (<https://doi.org/10.1039/D5SU00070J>). By linking pretreatment performance with techno-economic feasibility, this work



strengthens the case for ammonia as a cross-sector enabler of defossilisation. The purification of crude glycerol, a by-product of biodiesel production, is also used as a case study to compare the economic impact of multiple process models (<https://doi.org/10.1039/D4SU00599F>). The economic assessment is centre stage, incorporating sensitivity analyses that account for market volatility and feedstock variability, offering a commercially informed decision-making framework; however, a full LCA is not used. Instead, process-relevant sustainability-related key performance indicators (KPIs) are defined and used, such as heat and water requirement and CO<sub>2</sub> emissions. Together, these papers underscore the importance of TEA and sustainability assessment not as afterthoughts, but as core tools for developing and scaling renewable chemical processes.

## Bio-based product formulation

Stepping further along the value chain, the collection showcases how renewable feedstocks can be transformed into high-performance materials and functional additives. One study integrates ionosolv biomass fractionation with lignin fibre spinning to produce low-cost, sustainable carbon fibres, eliminating intermediate isolation steps and reducing emissions. This work advances lignin valorisation while also illustrating the role of techno-economic analysis and life cycle assessment in guiding materials innovation (<https://doi.org/10.1039/D5SU00218D>). Another study introduces a range of mono- and diesters synthesised from carbohydrate-derived 5-(chloromethyl) furfural *via* a renewable-compatible route. These molecules may serve as surfactants, fuel oxygenates, and plasticisers, expanding the molecular toolkit for functional bio-based formulations (<https://doi.org/10.1039/D4SU00563E>). Together, these studies highlight how alternative feedstocks can underpin the design of novel products essential to the transition away from fossil-derived chemicals.

## Systems integration and process modelling

Zooming out from individual technologies, this collection also considers how process innovations can be coordinated and scaled. A critical review provides a high-level meta-analysis of defossilisation routes for the chemical sector, combining energy and material flows in scenarios that jointly consider carbon sourcing, renewable energy, and hydrogen deployment (<https://doi.org/10.1039/D4SU00601A>). Crucially, it frames innovation not in isolation but as contingent on synchronised policy, regulatory, and societal support. Another study grounds these ideas in a detailed model for methanol and ammonia co-production, coupling green hydrogen and CCU inputs (<https://doi.org/10.1039/D4SU00647J>). Comparing 12 integration pathways through cradle-to-gate life cycle assessment, it identifies viable, flexible configurations that minimise environmental burdens. Together, these contributions emphasise the necessity of systems thinking to coordinate the energy, carbon and infrastructure transitions to make preceding innovations viable at scale.

## Chemical recycling and circularity

Closing the loop for carbon-based chemicals is a defining challenge, with articles in this themed collection examining complementary strategies to reinforce circularity and resource efficiency. An elegant example of waste valorisation is the conversion of pine needle biomass into a support for a high-performance, reusable Ni-nanoparticle catalyst for hydrogenation, which reduces dependence on scarce metals while embedding green chemistry principles. (<https://doi.org/10.1039/D5SU00026B>). A full-process perspective is also presented: integrating experimental biomass-to-isobutanol conversion through microbial fermentation with system level techno-economic analysis (<https://doi.org/10.1039/D4SU00283K>). Together, these works show that end-of-life valorisation and whole-system optimisation are critical tools in designing circular, economically competitive bio-based industries.

As the world pursues net-zero goals, the sector must phase out fossil carbon as an energy and chemical feedstock, and support sustainable, circular flows of carbon and other elements. We hope this collection provides readers with foundational knowledge and perspectives spanning molecular design to systems integration, supporting cross-sectoral dialogue about technical and policy innovations. We encourage researchers, practitioners, and policymakers to explore the collection and consider how the research within can inform future studies, policy, and practice.

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