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State of the Art in Thermal Catalytic Upgrading of Biomass and Biomass-Derived Intermediates

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Abstract

Biomass-derived energy sources represent a promising domestic route for fuel and chemical production, taking advantage of largely underutilized biological and waste resources. Heterogeneous catalysis plays a key role in these biomass conversion processes, as reflected by all American Society for Testing and Materials–approved pathways for producing sustainable aviation fuel proceeding through a catalytic step. This concise review seeks to establish the state of the art in thermal catalytic process development for various biomass-derived feedstocks and the current enabling capabilities that aid this development. Research needs are identified and described throughout the article, as further advancements in heterogeneous catalysis are required to improve the affordability and realize the full potential of biomass-derived products.

1. INTRODUCTION

A resurgence has been observed in the pursuit of converting biomass to fuels and chemicals, particularly in the heavy-vehicle transportation (i.e., aviation, trucking, marine) sector, for which the application of electrification is limited. Biomass-derived energy sources represent a pivotal component of future energy landscapes through their tremendous availability and flexibility to be processed into a wide range of fuels. This current resumption in the conversion of biomass to fuels is further reflected by 112 offtake agreements by airlines since 2020 involving the long-term purchasing of sustainable aviation fuels (SAFs) for use in air transport (1).

Offtake agreements: these agreements provide commitments to the supply and use of sustainable aviation fuels in the airline industry, helping reduce risks associated with developing these technologies

Sustainable aviation fuels (SAFs): jet fuels produced from renewable biomass or waste resources, which offer a lower carbon footprint alternative to traditional petroleum-derived fuels

Supplemental Material >

An array of biomass upgrading technologies have been developed, with heterogeneous catalysts playing a key role in many of these conversion processes (2–7). Catalyst development in this respect is inherently complex given the multifaceted nature of biomass feedstocks and the associated conversion technologies. Through a Sankey plot summarizing 402 catalytic biomass upgrading research articles published in 2023, **Figure 1** offers two takeaways about the state of catalytic biomass upgrading research. First, reaction strategies for generating products with similar properties can be quite diverse. For example, both diesel and aviation fuels consist of hydrocarbons (or ethers, in the case of diesel) with similar chain lengths ($C_{10–22}$ and $C_{9–15}$, respectively), but predominant research strategies to generate them are distinct. **Figure 1** shows that 63% of published diesel pathways involve carbon chain length–preserving reactions of a single feedstock (fats, oils, and greases), whereas aviation fuel pathways are proposed with 10 different feedstocks, no single one of which comprises more than 32% of the total, and the majority (77%) of pathways use C–C bond formation steps (see **Supplemental Data**). Additionally, a large portion of published research focuses on either improving methods to transform feedstocks to molecules with a similar structure (e.g., raw biomass catalytic pyrolysis to oxygenated oils; transformation of sugars or furfural and derivatives to furanics; and transformation of lignin and derivatives to oxygenated aromatics) or building upon already commercialized processes (e.g., esterification of fats, oils, and greases to biodiesel and Fischer–Tropsch reactions of syngas).

We seek to establish the state of the art in thermal catalytic process development for various biomass-derived streams, with an emphasis on emerging pathways to generate heavy-duty hydrocarbon fuels. We also highlight recent advancements in enabling capabilities across catalyst synthesis, characterization, and computational efforts, which have facilitated development in

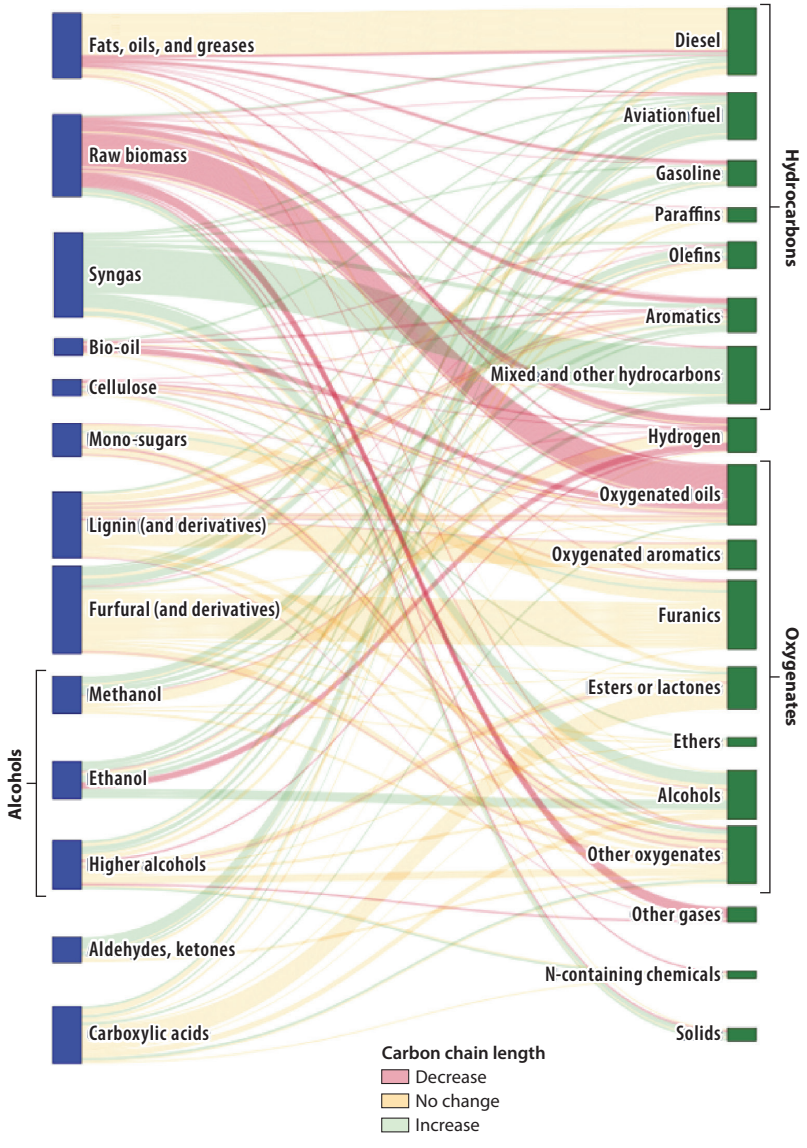

Figure 1

Feedstocks and products from scholarly research papers employing thermal catalysis for upgrading sustainable feedstocks published in 2023 (402 papers). Note: Articles found using SciFinder with search terms: alcohol, ethanol, propanol, butanol, carboxylic acid, volatile fatty acid, acetic acid, propionic acid, butyric acid, butanoic acid, pentanoic acid, valeric acid, hexanoic acid, caproic acid, octanoic acid, capric acid, levulinic acid, furfural, hydroxymethylfurfural, furan, lignin, syngas, methanol, pyrolysis, bio-oil, hydrothermal liquefaction, fat, oil, grease, aldehyde, ketone, sugar, glucose, fructose, sustainable fuel, and sustainable chemical. Articles were down-selected using the concepts of "catalysts" and "biomass" and the CA sections "catalysis, reaction kinetics, and inorganic reaction mechanisms" and "fossil fuels, derivatives, and related products." Here, carbon chain length refers exclusively to the length of C–C bond chains; reactions such as *trans*-esterification that alter only C–O and O–H bonds are categorized as not changing carbon chain lengths. Processing data for this figure have been included in **Supplemental Data**.

Supplemental Material >

this area. This timely review may aid in guiding future research and development. To retain the focus of this review, processes that have already been commercialized, as well as biorefining of lignin through reductive catalytic fractionalization and catalytic biomass gasification processes, are not included. For references on these topics, readers are directed to the Related Resources. Throughout the text, sidebars call out recent commercial activity in process development.

Diesel-range hydrocarbons: include a mixture of organic compounds typically ranging from 12 to 24 carbons (C_{10}–C_{24}) on average

Jet-range hydrocarbons: e.g., kerosene-type jet fuel, typical carbon range of approximately C_8 to C_{16}

2. CATALYTIC PROCESS DEVELOPMENT

2.1. Upgrading of Biochemical Intermediates

Within the broad discipline of catalytic upgrading for fuel and chemical production, one promising direction leverages intermediates derived from biochemical deconstruction of biomass or the biological conversion of wet wastes. These approaches can be directly coupled with the upgrading of liberated sugars or molecules produced from waste-derived sugars or other biomass components via microbial upgrading routes. These biochemical intermediates can ultimately be upgraded through diverse catalytic processes to produce finished fuel blendstocks or high-value biochemical products. Such an approach requires upstream processes including biochemical deconstruction of biomass and fermentation routes to facilitate conversion of complex substrates into singular or at least simplified intermediates to enable high-efficiency catalytic conversion.

Within this paradigm of upgrading of biochemical intermediates, myriad diverse molecules have been produced or could be produced biologically. A few examples of classes of potential intermediate molecules include alcohols, sugars, acids, aromatics, ketones, esters, lipids, and aldehydes. In this section, the focus is narrowed to three independent routes that have demonstrably high potential for the synthesis of diesel- and jet-range hydrocarbons: ethanol and other alcohols, volatile fatty acids, and furans.

2.1.1. Ethanol and alcohols. This section focuses on the upgrading of C_{2+} alcohols to jet- and diesel-range hydrocarbons. Subsequent processing produces either a drop-in fuel[1] (i.e., diesel) or fuel blendstock (i.e., jet). Emphasis is placed on converting ethanol, as it is presently the most common biomass-derived liquid (~60 million metric tons/year in the United States alone). However, similar processing can be used for higher alcohols (C_{3+}), particularly 2,3-butanediol (BDO) (8) and butanol (9), which are highlighted herein. Development of commercial processes for ethanol–to–jet fuel production are discussed further in the sidebar titled Progress in Ethanol–to–Jet Fuel Commercialization.[2]

PROGRESS IN ETHANOL–TO–JET FUEL COMMERCIALIZATION

Near-commercial processes that exist for ethanol-to-jet production rely on ethanol dehydration, oligomerization, hydrotreatment, and distillation. For example, LanzaJet recently commissioned a commercial plant in Soperton, Georgia, to produce 10 million gallons of sustainable aviation fuel and renewable diesel per year from ethanol (205). Axens and Gevo (206) and Honeywell UOP (207) have also announced offerings for similar technology. Commercial technology for isobutanol-to-jet fuel also exists, employing isobutanol dehydration, oligomerization, hydrotreatment, and distillation (208). However, the routes mentioned above involving an acetaldehyde intermediate have been reported only at the bench scale.

[1]The use of biofuels as drop-in fuels requires that the produced hydrocarbon mixture is fully compatible with and be used as a blended component of petroleum within current infrastructures.
[2]Ethanol-to-jet fuel production commercialization offers a diversification strategy for ethanol producers.

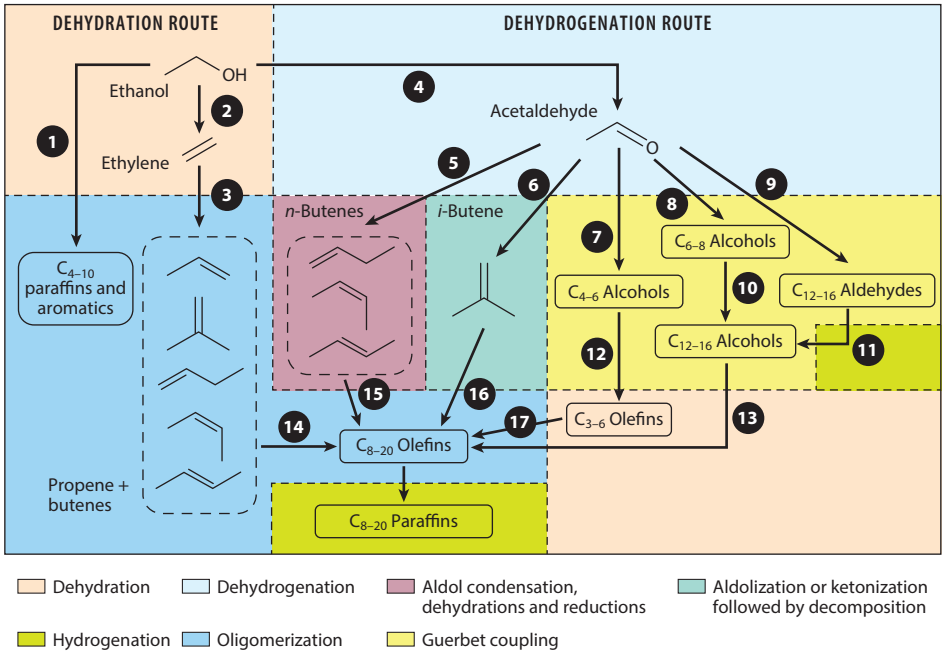

Figure 2

Overview of catalytic routes of converting ethanol into jet- and/or diesel-range hydrocarbons.

2.1.1.1. Fundamental chemistry. Conversion of ethanol into jet- and diesel-range hydrocarbons relies on reactions including dehydration (to olefins), dehydrogenation (to aldehydes), hydrogenation (of C=C and C=O bonds), acid-catalyzed olefin oligomerization, metal-catalyzed olefin oligomerization, aldolization, and ketonization (**Figure 2**). Two primary approaches are used for upgrading C_{2+} alcohols, dictated by the initial C–C bond formation, illustrated for ethanol in **Figure 2** by pathways 1 and 2 to 3. First, alcohols can be dehydrated into olefins of the same carbon number using acid catalysts (**Figure 2**, pathway 2). Produced olefins then can be oligomerized into higher olefins using acid catalyst and/or transition metal complexes (**Figure 2**, pathway 3). Second, alcohols can undergo dehydrogenation over metal catalysts, forming an aldehyde intermediate (**Figure 2**, pathway 4). For example, ethanol can be dehydrogenated into acetaldehyde for subsequent upgrading into fuel-range hydrocarbons (**Figure 2**, pathways 5–9 and subsequent reactions).

Once formed, acetaldehyde can be converted into various intermediates via combinations of condensation, ketonization, dehydration, and hydrogenation reactions. For example, acetaldehyde can undergo condensation, using acid catalysts, followed by hydrogenation, using metal catalysts, to form either C_{4+} aldehydes (after C=C hydrogenation) or C_{4+} alcohols (after C=C and C=O hydrogenation), as shown in **Figure 2**, pathways 5–11. Higher alcohols can undergo further chain growth (with the extent of growth governed by process conditions) via Guerbet coupling (**Figure 2**, pathways 7–10). Alternatively, ethanol can be converted into higher olefins (C_{3+}) directly using multifunctional catalysts (10–13). For example, ethanol to *i*-butene formation occurs via a sequence of reactions including dehydrogenation, ketonization, condensation, dehydration, and decomposition over balanced mixed oxide catalysts. Near-maximum theoretical yield to *i*-butene can be reached over catalysts such as $Zn_xZr_yO_z$ when operated at 475°C and ambient pressure under a steam-to-carbon ratio of 2.5 cofed with N_2 (14). Ethanol also can be converted

directly into *n*-butene via another sequence of reactions that includes dehydrogenation, condensation, hydrogenation, and dehydration over metal-promoted mixed oxides in H_2 at 325–400°C at pressures of 1–7 bar to achieve olefin yields of 85% (10, 12, 13). The latter mechanism avoids the ketonization step, thereby circumventing carbon loss via stoichiometric CO_2 formation. Also of note, upon crotonaldehyde formation—on route to *n*-butene—a bifurcation in the mechanism has been reported. Crotonaldehyde undergoes Meerwein–Ponndorf–Verley reduction to form crotyl alcohol, which can undergo subsequent dehydration (to butadiene) and selective hydrogenation (to *n*-butene) (13). Alternatively, crotonaldehyde can undergo hydrogenation and isomerization, thereby forming 1-butanol, which can dehydrate to *n*-butene. Dagle et al. (13) suggested the latter mechanism is preferred because it avoids formation of butadiene intermediate, which is a coke precursor. Catalysts comprising different combinations of acid and metal sites and process conditions can be tuned to favor the different reaction mechanisms and for ease of regeneration (15).

The conversion of higher alcohol BDO into butene is a promising route for producing SAFs due to BDO's low toxicity and high fermentation titers. Challenges with BDO's separation, arising from its high boiling point and hydrophilicity, were overcome with a new approach using dioxolane formation from aldehydes (which phase separates from fermentation broth) (16), followed by catalytic conversion over Cu/ZSM-5 to maximize C_{3+} alkene yields to 96% (17). This method offers improved selectivity over direct BDO conversion, demonstrating a scalable pathway for producing alkene-rich SAF precursors.

With all routes, a key processing component includes olefin oligomerization to diesel- and/or jet-range hydrocarbons. Nickel-based catalysts supported on silicates or aluminosilicates typically are used for ethylene oligomerization (18). Non-nickel-containing solid catalysts can be used to oligomerize higher olefins. The oligomerization distribution typically is described by the Schulz–Flory product distribution and therefore is relatively nonselective to products of a specific length. This limitation makes it difficult to selectively produce jet- and diesel-range hydrocarbons (19). It may be overcome by performing oligomerization in multiple stages. Once diesel- and/or jet-range olefins, aldehydes, and/or aromatics are formed, they are hydrogenated and distillated into either drop-in or blendstock fuels. For more detail on the chemistries and processes for ethanol conversion into middle distillate fuels, readers are directed to Eagan et al.'s (19) excellent review. Several recent reviews have detailed the catalysts and processes used in the upgrading of ethanol to value-added chemicals (20–22).

2.1.1.2. State-of-the-art comparison. Realizable distillate yields of current technologies range from approximately 25% for single-stage systems to near unity for condensation-based routes through acetaldehyde or dehydration-oligomerization routes through ethylene, shown in **Figure 2** (19). The degree of process intensification required to increase yield to distillate is the major trade-off to be made for potential adoption of systems currently in bench-scale development. Single-stage systems that combine ethanol dehydration and oligomerization over acid catalysts are limited by statistical product distribution. Distillate formation through isobutene places the maximum theoretical yield at 65% due to the formation of CO_2 during ketonization. Aldolization routes, however, do not have theoretical limits on high yields to distillates. The following section addresses catalytic improvements needed to actualize high distillate yields upon subsequent separation, hydrogenation, and oligomerization.

2.1.1.3. Research needs. Despite the commercial progress of ethanol-to-fuels pathways, several technical challenges persist. For example, understanding how to tune olefin oligomerization toward more linear instead of branched hydrocarbons is a classic challenge in heterogeneous

catalysis, and such improvements could lead to improved fuel quality for high-cetane diesel (19).[3] Also, producing cycloalkane-rich jet blendstocks could lead to improved energy density (23), which is an attractive performance enhancement for commercial airliners. Additionally, alternative routes relying on aldolization also may lead to process improvements. For example, ethanol dehydration is endothermic and requires relatively large amounts of energy to drive the reaction (24). Coupling endothermic dehydrogenation and exothermic condensation reactions, using routes through acetaldehyde as described above, presents the opportunity for energy savings. However, these catalytic pathways use multifunctional catalysts that typically incur undesirable side products (e.g., small amounts of light alkanes and oxygenates). Increasing selectivity by using improved catalyst designs could enhance carbon efficiency, which is critical to the process economics and overall realizable yield to distillates. In contrast, higher alcohols, such as 2,3-BDO, can achieve higher carbon efficiency with fewer reaction steps and less complexity (17). However, they face challenges as emerging processes, including the higher costs associated with fermentation compared to established ethanol processes. Further, catalyst stability for these processes must be improved to facilitate commercial adoption.

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2.1.2. Carboxylic acids. This section focuses on upgrading of short-chain ($C_{2–8}$) monocarboxylic acids to hydrocarbons, because acids could be produced biologically from waste at substantial scales (~70 million tonnes/year in the United States alone) (25) at low cost. Firstly, other near-commercialized or promising carboxylic acid–upgrading pathways are acknowledged. Triglyceride-derived long-chain fatty acids ($C_{12–26}$ monocarboxylic acids) and their ester derivatives are already commercial components or feedstocks for biodiesel and SAF (three American Society for Testing and Materials–approved SAF pathways use hydrotreated fatty acids); they also have soap, surfactant, and lubricant applications (26–28). Fermentation of biomass-derived sugars or lignin can also produce molecules such as dicarboxylic (e.g., itaconic, muconic) or other oxygen-functionalized (e.g., lactic, levulinic) acids, which can be upgraded via selective hydrogenation (29), dehydration (30), decarboxylation (31) to polymer precursors, or combinations thereof.

2.1.2.1. Fundamental chemistry. **Figure 3*a*** provides a summary of catalytic upgrading strategies for $C_{2–8}$ monocarboxylic acid pathways to hydrocarbon fuels and chemicals. The chain lengths of hydrocarbons in heavy-duty fuels (jet: $C_{8–16}$; diesel: $C_{10–22}$) are higher than those of relevant carboxylic acids, so catalytic upgrading strategies commonly include both chain elongations and reductions (deoxygenations), often carried out in sequential reactors. Carboxylic acid upgrading strategies start with either (*a*) selective reduction to alcohols ($RCOOH+2H_2 \rightarrow RCH_2OH+H_2O$), (*b*) ketonization ($RCOOH+R'COOH \rightarrow R(C=O)R'+H_2O+CO_2$), or (*c*) transformation to olefins and aromatics. The first two chemistries are single stoichiometric reactions, whereas the third encompasses many sequential reactions (including the first two). Selectivity is maximized by limiting C–C cracking and overreduction. Metal alloying prevents these reactions during alcohol formation, whereas amphoteric oxides maximize ketonization selectivity. Huq et al. (32) showed that ketones can either be hydrotreated to alkanes over commercial supported metal catalysts or, if their chain lengths are still too short for the desired application, undergo aldol condensation over solid acids such as Nb_2O_5 or $MgAlO_x$ (33) with subsequent hydrotreatment. Alkenes formed from acid upgrading or alcohol dehydration can be oligomerized and hydrotreated to form desired alkane fuel products through commercialized processes.

[3]Higher cetane ratings for diesel fuels correspond to enhanced combustion efficiency, an important descriptor of fuel quality.

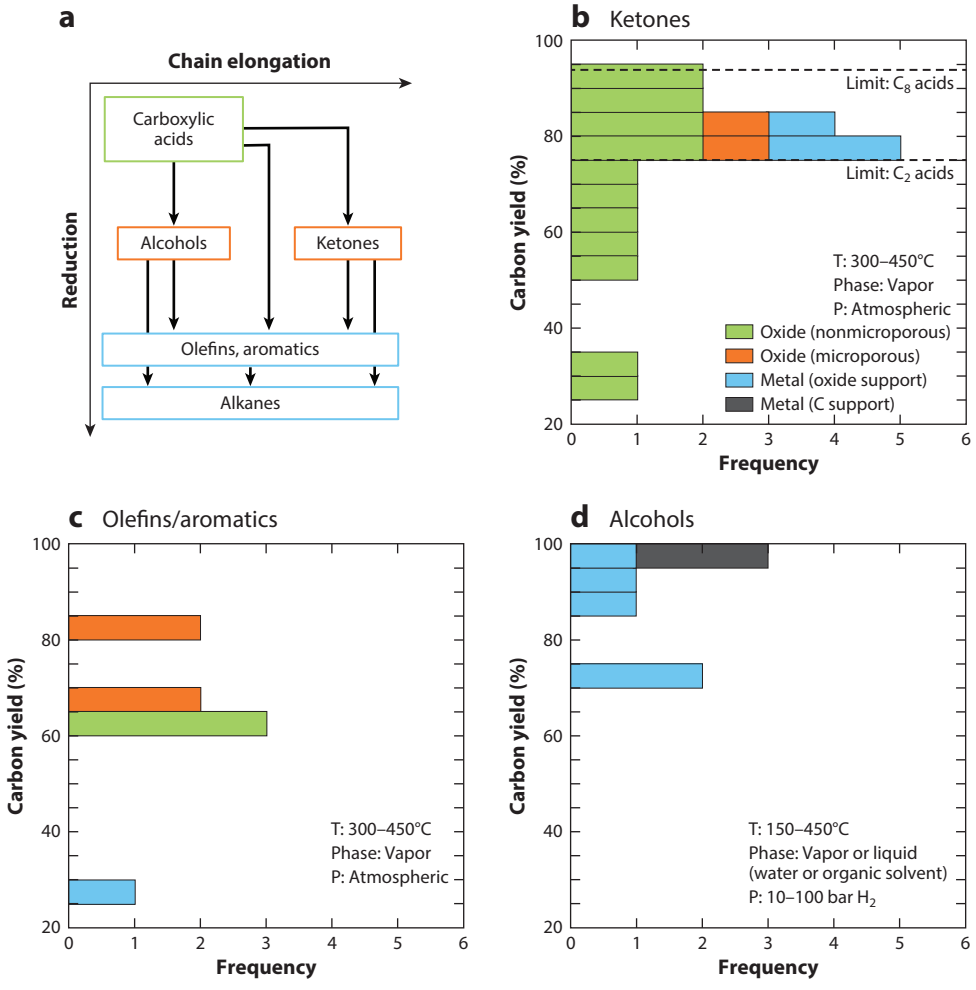


Figure 3

Overview of the state of the art in $C_{2–8}$ monocarboxylic acid upgrading. (*a*) A conceptual map of catalytic acid reduction and C–C bond elongation pathways. (*b–d*) Carbon yields of catalytic acid upgrading to form (*b*) ketones, (*c*) olefins/aromatics, and (*d*) alcohols and reaction condition ranges reported in academic literature since 2015.

2.1.2.2. State-of-the-art comparison. All reactions mentioned above have been demonstrated in continuous reactors at lab scale, an important step toward scale-up, apart from condensations of non-methyl ketones. Sun et al. (34) noted that these ketones are particularly hard to activate due to either steric hindrance of H-atoms adjacent to the carbonyl group or increased coking propensity. Each of the three initial acid-upgrading reactions has specific advantages (e.g., ketonization and olefin/aromatic formation are performed without H_2 addition), and some intermediates may be desirable over others for specific use cases (e.g., $C_{6–8}$ aromatics are valuable chemical precursor coproducts). **Figure 3*d*** compares carbon yields and process conditions of the pathways reported in recent (since 2015) open literature. Carbon yields from ketonization, as shown in **Figure 3*b***, are close to the stoichiometric limit, but CO_2 loss inherent to this reaction constrains yields to lower than unity. **Figure 3*c*** shows that carbon yields of acids upgrading to alkenes or aromatics

are also much lower than unity; side reactions of C–C scission to light alkanes or alkenes are significant. Reduction of carboxylic acids to alcohols is uniquely selective among these pathways, with several studies reporting carbon yields at or near 100% over carbon- or metal-supported catalysts (**Figure 3*d***).

2.1.2.3. Research needs. Multifunctional catalysts capable of performing sequential upgrading steps with high selectivity would allow for fewer upgrading unit operations. However, **Figure 3*c*** shows that such efforts for olefin and aromatic formation have had limited success thus far due to high cracking selectivity. Practical catalysts must also be developed. Ketonization and olefin/aromatic formation catalysts are already inexpensive oxides or zeolites, but highly selective alcohol synthesis catalysts currently require rare earth metals [Ru (35), Re, Pt (36)] or complex supports such as ultrathin graphene nanoparticles (37).

From the process development perspective, the cost and energy inputs from production and separation of carboxylic acids, which Huq et al. (32) found to comprise nearly 85% of CO_2 emissions for production of SAFs from food waste, must be attenuated via implementation of advanced strain development, separations, and process integration. Additionally, possible catalyst and reactor degradation caused by biogenic impurities must be understood and resolved through catalyst or equipment design. Engineering-form catalysts must also be tested on stream for commercially relevant times on stream (~4,000 h) to identify long-term deactivation modes and analyzed for potential mass and heat transfer limitations, as Miller et al. (38) demonstrated for ketonization over ZrO_2.

2.1.3. Furans. This section explores the transformation of furfurals [furfural and 5-hydroxymethylfurfural (HMF)] into hydrocarbons in the range of $C_{9–16}$. Furfural and HMF produced from C_5 and C_6 sugars, respectively, are recognized as key platform molecules to produce fuels and chemicals. By leveraging these intermediates, the strategy for C–C chain elongation involves aldol condensation followed by hydrodeoxygenation (HDO) to yield hydrocarbons suitable for blending into jet and diesel fuel.

2.1.3.1. Fundamental chemistry. **Figure 4*a*** illustrates a catalytic strategy for upgrading furfurals to hydrocarbon fuels. Furfural and HMF are short-chain ($C_{5–6}$) dehydrated products of biomass-derived sugars obtained under aqueous acidic conditions. Sugar conversion efficiencies greater than 90%, and furfural/HMF yields between 60% and 90%, have been reported at temperatures ranging from 160°C to 200°C, with reaction times ranging from 30 min to several hours, depending on the desired conversion efficiency and the product yield and stability (39–41). Both homogeneous and heterogeneous acid catalysts in batch and continuous reactor systems are employed for the dehydration reactions. Homogeneous catalysts often include mineral acids such as sulfuric or hydrochloric acid. In contrast, heterogeneous catalysts can consist of materials like zeolites or amorphous silica alumina, sulfonated carbons, mixed-metal oxides, and ion-exchange resins, which have demonstrated effectiveness for this pathway (42, 43). Because furfurals lack enolizable α-hydrogens, their cross-aldol condensation must occur with ketones containing enolizable α-hydrogens and a carbonyl group (44, 45). The aldol chemistry of furfurals with various ketones demonstrates that ketones with shorter carbon chains exhibit higher reactivity compared to those with longer chains. Moreover, short reaction times and a ketone-to-furfural molar ratio greater than 1:1 favor the formation of mono-adducts in the $C_{8–11}$ range, which are suitable for jet fuel. Conversely, extended reaction times and a furfural-to-ketone molar ratio greater than 1:1 result in di-adducts with chain length exceeding C_{13} (based on the carbon atoms in the ketone), which are suitable for diesel fuel (46–49). Long-chain paraffinic fuels are ultimately obtained through the HDO of chain-elongated oxygenates. The HDO chemistry of aldol adducts involves three major paths: (*a*) hydrogenation of C=C and C=O groups, (*b*) ring-opening of furanic rings via cleavage

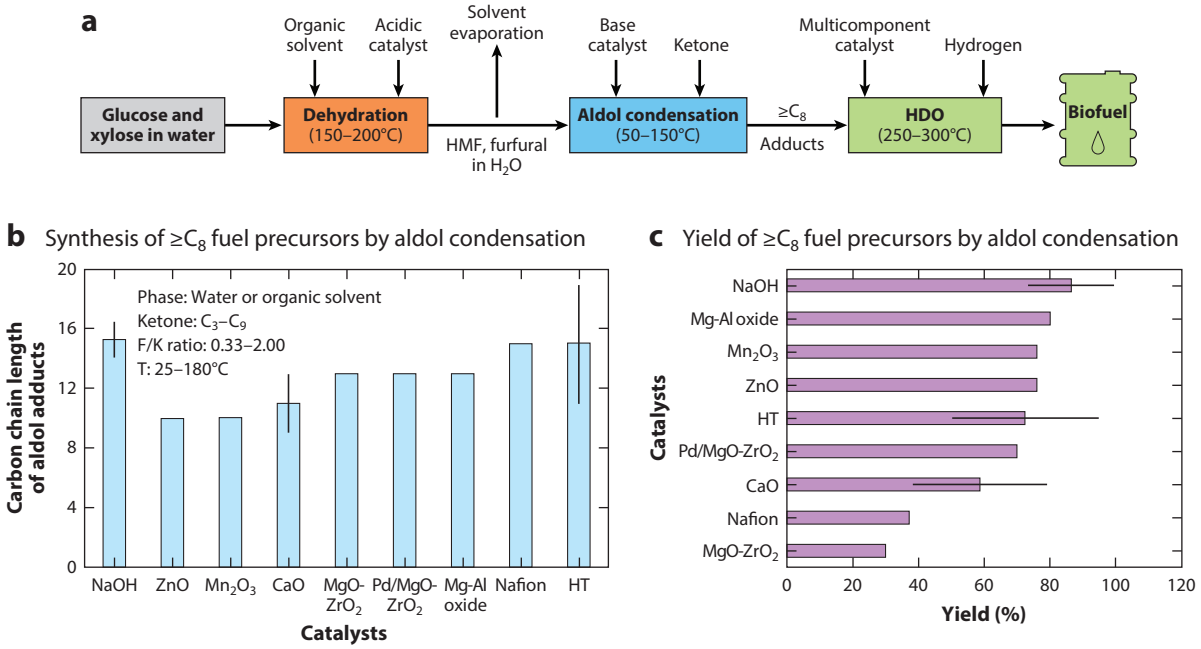


Figure 4

Overview of the state of the art for upgrading furfurals to hydrocarbons. (*a*) A conceptual process overview, highlighting the critical steps involved in upgrading mixed sugars into hydrocarbons through aldol condensation reactions. (*b*,*c*) The impact of catalyst type on chain length and yield ranges of ≥C8 fuel precursors produced via aldol condensation performed under varied reaction conditions. The chain length and yield ranges of fuel precursors, as reported in the literature (46, 51, 52), are depicted with standard deviations for selected catalysts. Abbreviations: F/K, furfural-to-ketone ratio; HDO, hydrodeoxygenation; HMF, 5-hydroxymethylfurfural; HT, hydrotalcite.

of C–O–C bonds, and (*c*) deoxygenation through the removal of oxygen in the form of water by breaking of C–O bonds in the open-chain intermediates (50).

2.1.3.2. State-of-the-art comparison. Recent advancements in catalytic processes for the transformation of furans into diesel and jet fuel range adducts have focused predominantly on solid base catalysts in aldol condensation reactions. Among the base catalysts, layered double hydroxide and combinations of MgO with Al_2O_3 (hydrotalcite) and ZrO_2 have emerged as highly active catalysts under aqueous conditions (53). However, layered double hydroxides and hydrotalcite require intricate pretreatments to generate strong basic sites, and their regeneration poses challenges. Additionally, hydrotalcite exhibits slightly lower activity compared to MgO-ZrO_2. The high concentration of base sites on the surface of MgO-ZrO_2 was the prime factor for its superior performance, although the aldol condensate yield was low in repeatability testing. Faba et al. (54) improved the composition of MgO-ZrO_2 catalysts by incorporating Pd into the framework or doping onto high–surface area graphite and carbon nanofibers to counteract selectivity losses during consecutive aldol runs.

Figure 4*b*,*c* compares the influence of different catalyst types on the chain length and yield ranges of ≥C_8 fuel precursors produced via aldol condensation under various process conditions reported in the literature (46, 51, 52), highlighting the carbon chain length of aldol adducts obtained. **Figure 4*c*** shows that yields approaching 80%, similar to those achieved with NaOH, can be replicated with heterogeneous catalysts. HDO of aldol adducts has been demonstrated

extensively and relies predominantly on noble metal catalysts with acidic sites. Catalysts such as Pd/Al_2O_3, Pt/Al_2O_3, Pd/C, and Ru/hydroxyapatite have shown limited production (30%) of long-chain hydrocarbons. The incorporation of secondary active sites (e.g., Pd/C+ phosphotungstic acid, Ru/hydroxyapatite+ZSM-5, Pd-FeO_x/SiO_2, Pd/Al_2O_3+$NbOPO_4$, Pt/SiO_2-Al_2O_3) has significantly enhanced HDO activity. These advancements have led to yields of ≥90% long-chain hydrocarbons under reaction conditions of 250–300°C for 3–24 h, with H_2 pressures ranging from 30 to 100 bar (49, 55–60).

2.1.3.3. Research needs. Heterogeneous catalysts, commonly used in aldol condensation of furans, could potentially deactivate due to impurity and byproduct deposition and catalyst phase changes in aqueous environments (61).[4] To mitigate these issues, research should prioritize the optimization of engineered catalysts by adjusting surface properties, such as hydrophilicity/hydrophobicity, to resist byproduct deposition. Additionally, given that furans are produced in acidic media, the development of effective acidic aldol condensation catalysts is imperative to avoid neutralization and purification costs (62, 63). Similarly, numerous catalysts have been tested for aldol-adduct HDO. Costly noble metal–based multicomponent catalysts containing acidic sites have been identified as the most active, but they often face rapid deactivation and recycling challenges. Hence, efforts should be directed toward developing stable and long-life non-noble metal catalysts using advanced technologies such as single-atom, bimetallic, or multi-metallic alloys. Moreover, a systematic attempt should be explored to evaluate the suitability of current commercial sulfide hydrotreating catalysts.

To improve market competitiveness, novel and robust strategies must be devised that can improve the cost effectiveness of biorefineries that would manufacture furan-based biofuels as the only product stream, as reflected by techno-economic analyses (64). Hence, future research should explore coproduction of industry-relevant products (e.g., fine chemicals, lubricants) and simultaneously search for long-life heterogeneous catalysts. Furthermore, establishing efficient and economic separation protocols to purify target products will be indispensable. In summary, aligning the process with real-time applications will require exploring practical value-added applications and carefully selecting extractants, reaction solvents, and catalysts.

2.2. Syngas and C1 Conversion

This section focuses on recent advancements in the upgrading of syngas, a mixture of CO and H_2, and related C_1 building blocks, CO_2 and methanol. Despite decades of research devoted to the upgrading of these light oxygenates, and the commercial practice of Fischer–Tropsch synthesis, there remains a continued interest in the development of new catalytic pathways from C1 oxygenates to various hydrocarbons—olefins, aromatics, and fuel-range paraffins. This catalyst and process science is motivated by (*a*) the desire to use the variety of renewable and waste carbon-based feedstocks that can be gasified to provide syngas, (*b*) the rise in carbon-capture technologies that can provide clean CO_2 feedstocks, (*c*) the desire to develop catalytic technologies that are economically feasible at smaller scales to use these distributed resources, and (*d*) the ability to tune the hydrocarbon products via catalyst design and process conditions to target valuable fuels and chemicals. Given the breadth of feedstocks, catalytic chemistries, process designs, and target products, the interested reader is referred to recent review and perspective articles that focus on specific aspects of syngas and C1 upgrading (65–68). Here, the state of the

[4]Deposited byproducts (including polymers and humins) produced by undesired side reactions can lead to a significant decrease of catalyst lifetime and selectivity, requiring regeneration to overcome.

art for process intensification approaches is presented for multicomponent catalysts starting from CO and/or CO_2 that target fuel-range hydrocarbons (69).

OX-ZEO: oxide-zeolite catalyst system, combines hydrogenating capability of metal oxide with zeolite acid sites for syngas to hydrocarbon conversion

2.2.1. Fundamental chemistry. One attractive design in a process intensification strategy starting from CO or CO_2 is to proceed through a methanol or dimethyl ether intermediate, where the chemistry from CO or CO_2 to methanol can be accomplished with a commercial Cu–Zn–Al mixed oxide (CZA), and the conversion from methanol to dimethyl ether is achieved by a simple acid catalyst, such as gamma-Al_2O_3 (68–71). As noted in point *d* above, the subsequent methanol-to-hydrocarbons (MTH) chemistry can be controlled by the choice of hydrocarbon synthesis catalyst (typically a Brønsted acidic zeolite, zeotype, or metal-modified zeolite/zeotype) and reaction conditions. The series of reactions, including the important water–gas shift reaction that is relevant if starting from CO_2, are shown in Equations 1–4, using butane as an example hydrocarbon product. However, a critical design challenge emerges when considering a multifunctional or multicomponent catalyst to directly convert CO or CO_2 to hydrocarbons in this cascade chemistry: mismatched reaction conditions for the series of reactions. Matching the reaction temperatures for methanol synthesis and MTH is particularly problematic because lower temperatures (200–250°C) typically are employed for methanol synthesis, but high temperatures (>350°C) are used for MTH reactions.

$$CO + 2H_2 \leftrightarrow CH_3OH \quad 1.$$

$$2CH_3OH \leftrightarrow CH_3OCH + H_2O \quad 2.$$

$$2CH_3OCH_3 + H_2 \rightarrow C_4H_{10} + 2H_2O \quad 3.$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad 4.$$

2.2.2. State-of-the-art comparison. The mismatched reaction conditions for the series of reactions from CO or CO_2 have been addressed in two ways: developing high-temperature methanol synthesis catalysts to work with high-temperature MTH catalysts or employing the traditional methanol synthesis catalyst and developing a low-temperature MTH catalyst. When seeking to compare catalyst performance, a wide range of CO or CO_2 conversions are found in the literature. Based on the focus here, a suggested relevant comparison is fuel-range hydrocarbon selectivity. Notable success using a high-temperature CO conversion catalyst was attained using the OX-ZEO process, in which a mixed-metal oxide catalyst (e.g., $Zn_2Mn_1O_x$) is combined with large-pore zeolites. Operating at relatively high temperature and pressure (360°C, 4 MPa), this route may proceed through ketene rather than methanol (72), but nevertheless, it yields gasoline-range products with high C_{5-11} selectivities (63–76%) (73, 74). Alternatively, Pd-based high-temperature methanol synthesis catalysts have also been paired with traditional zeolite MTH catalysts (e.g., H-ZSM-5) to generate fuel-range hydrocarbons under similar conditions of 310–375°C and 2–6 MPa (75, 76). Conversion of CO_2 with H_2 to gasoline-range hydrocarbons at nearly 80% selectivity to C_{5+} hydrocarbons has been achieved using modified CZA with zeolites (77). For the second approach using a lower-temperature MTH catalyst, high selectivities to C_{4+} hydrocarbons (~96% among hydrocarbon products) was reported for feeds of syngas, CO_2-rich syngas, and CO_2 with H_2 by employing stacked-bed, multicomponent catalysts employing a Cu-modified BEA zeolite (69, 70). These reports highlight recent success in achieving high selectivity to fuel-range hydrocarbons by employing a process intensification approach through methanol with multicomponent catalyst systems.

2.2.3. Research needs. Considering catalyst development, the traditional MTH zeolite catalysts are well-understood within the fuels/refining industry, from supply chain through operation

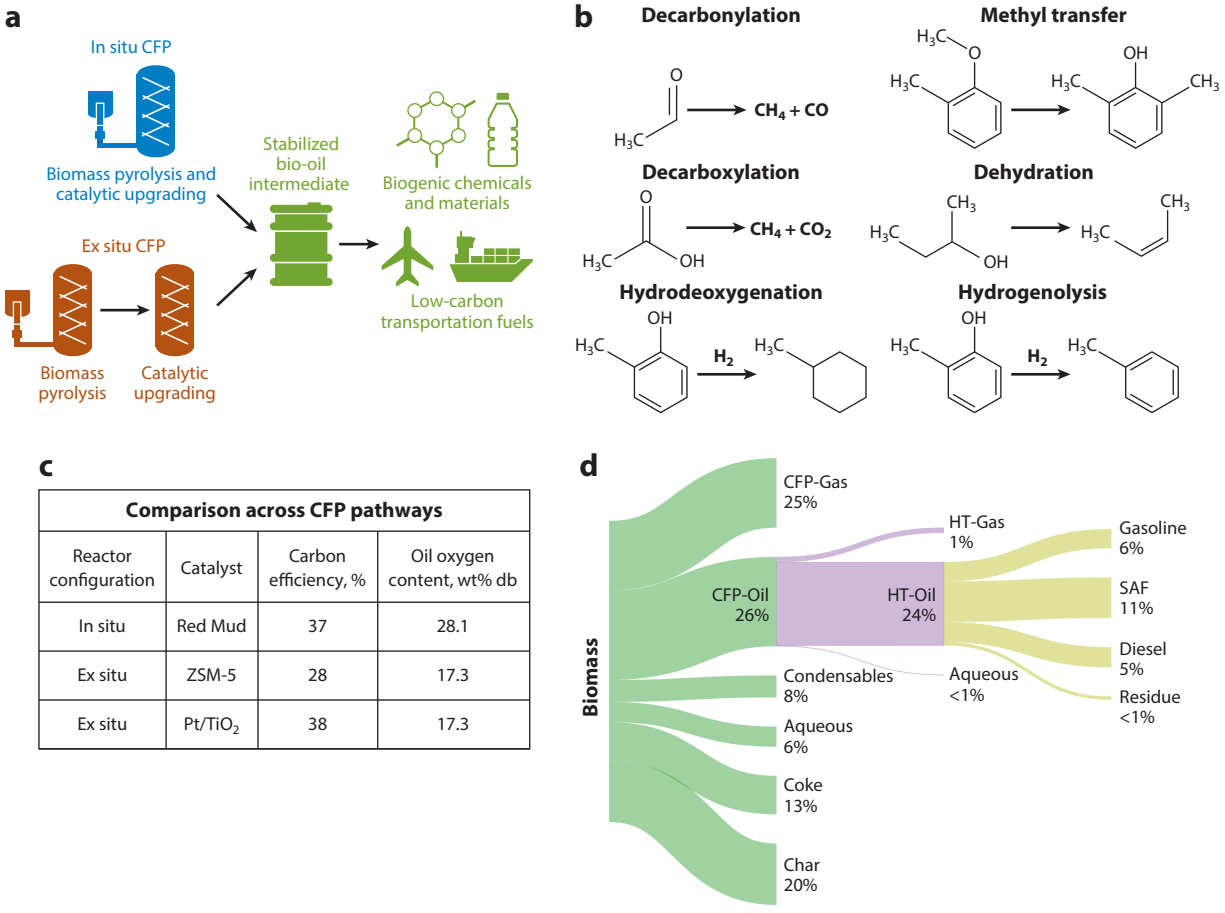
and regeneration; therefore, fewer research needs are associated with those materials. However, even a relatively simple metal modification, such as Cu-modified BEA zeolites, raises questions around catalyst stability at extended times on stream due to potential metal sintering or migration. Thus, translation of the promising performance with powdered research catalysts to engineered, formed materials is a critical first step, followed by performance testing at extended times on stream. Regeneration strategies must then be explored, because multicomponent catalysts present a challenge to regenerate the catalyst system without adversely affecting one of the components. For example, one cannot simply oxidize deposited carbon from a zeolite catalyst if it is mixed with CZA, which would irreparably deactivate at high temperatures with oxygen. Renewable and waste feedstocks often contain different impurities (or the same impurities but at different concentrations) than traditional feedstocks. Research into the sensitivity of specific impurities is needed to inform syngas/CO_2 cleanup requirements to ensure that high-quality gas is fed into the conversion reactor. Finally, industrial adoption of new processes requires many stage gates, often at intermediate scales. A recent report details the development of the methanol-to-olefins process (78), perhaps providing a blueprint for how to advance emerging processes with high fuel-range hydrocarbon selectivity beyond the lab scale with extended time-on-stream studies.

2.3. Catalytic Fast Pyrolysis

Catalytic fast pyrolysis (CFP) of biomass is a direct liquefaction process that includes a vapor-phase upgrading step to improve the quality and stability of the resulting bio-oil (79–85). CFP is a highly flexible platform that is compatible with a variety of lignocellulosic feedstocks and can be performed in either in situ or ex situ reactor configurations (86) (**Figure 5*a***).[5] For in situ CFP, pyrolysis and catalytic upgrading occur in a single reactor, which is advantageous in terms of the comparatively low capital requirements (87–92). During ex situ CFP (93), catalytic upgrading occurs in a dedicated downstream reactor, which enables independent optimization of reaction conditions and reduces catalyst exposure to potentially deactivating biomass impurities (94). In both cases, CFP is conducted near atmospheric pressure, differentiating it from hydropyrolysis, in which hydrogen pressures of up to 4 MPa are used. For all approaches, CFP enables the generation of bio-oil with reduced oxygen content, increased heating value, enhanced hydrocarbon miscibility, lower acidity, and improved thermal stability compared to noncatalytic pyrolysis oil (95). The improved properties of CFP oil reduce the risks associated with fouling and plugging during downstream hydroprocessing (*vide infra*, Section 2.5), which opens opportunities to generate high-quality fuel blendstocks for difficult-to-decarbonize (e.g., aviation and marine) transportation sectors (96, 97).

2.3.1. Fundamental chemistry. CFP can be performed under inert conditions or in the presence of co-fed hydrogen (89, 98, 99). Under inert conditions, metal oxide catalysts such as zeolites (100–103), γ-alumina (99, 104), and red mud (90, 105) have been used due to their low cost and ability to produce fuel-range hydrocarbons through decarbonylation, decarboxylation, dehydration, and methyl transfer reactions (**Figure 5*b***). Recirculating bed reactors are typically used with these catalysts to enable frequent oxidative regenerations due to rapid coking. This approach is effective in restoring catalyst activity, but the high coke rate reduces carbon efficiency to bio-oil, and the use of moving beds accelerates mechanical catalyst attrition (106). An alternative strategy involves the use of co-fed hydrogen coupled with metal–acid bifunctional catalysts (e.g., Pt/TiO_2, Mo_2C) (3, 107, 108). The addition of hydrogen increases process complexity. However, it also

[5]During CFP, catalyst activity can be maintained and restored by limiting catalyst contact times and minimizing high temperature regenerations for coke removal.



Comparison across CFP pathways

Reactor configuration	Catalyst	Carbon efficiency, %	Oil oxygen content, wt% db
In situ	Red Mud	37	28.1
Ex situ	ZSM-5	28	17.3
Ex situ	Pt/TiO_2	38	17.3

Figure 5

(*a*) A simplified process flow diagram outlining the conversion of biomass via in situ and ex situ CFP, (*b*) representative chemical transformations depicting some of the reactions that occur during catalytic upgrading of pyrolysis vapor under inert conditions and in the presence of co-fed hydrogen, (*c*) a comparison of carbon efficiency and oil oxygen content for different CFP reactor configurations and catalyst types (95), and (*d*) a Sankey plot mapping the carbon efficiency for an integrated CFP and hydrotreating process. Non-normalized yield data are from ex situ CFP using a zeolite catalyst, and derivations from 100% are due to material losses. Abbreviations: CFP, catalytic fast pyrolysis; HT, hydrotreated; SAF, sustainable aviation fuel. Image made with SankeyMATIC (CC BY 4.0).

enables a more diverse slate of chemistries, including hydrogenation, hydrogenolysis, and HDO, that can increase carbon efficiency by reducing coking and eliminating oxygen as water instead of carbon-containing light gasses (e.g., CO, CO_2) (98) (**Figure 5*c***). The lower coke rate also opens opportunities to use fixed bed reactors in a swinging bed configuration, which can extend catalyst lifetimes by reducing attrition (109, 110).

2.3.2. State-of-the-art comparison. The end-to-end production of hydrocarbon fuels from biomass via CFP and hydrotreating has been demonstrated through a series of bench-scale experimental campaigns using realistic biomass feedstocks and technical catalyst formulations (3, 96, 102, 107). A direct comparison between ex situ CFP with a zeolite catalyst under inert conditions, ex situ CFP with Pt/TiO_2 under HDO conditions, and in situ CFP with a red mud catalyst has also

been performed, using a common feedstock to enable benchmarking across the three approaches (95) (**Figure 5*c***). The highest CFP carbon efficiency was observed from the ex situ pathway with Pt/TiO_2 (38%), which also exhibited the lowest CFP oil oxygen content (17.3 wt%). In situ CFP with a red mud catalyst exhibited a similar carbon efficiency (37%). However, it produced a CFP oil with a comparatively high oxygen content (28.1 wt%). Ex situ CFP with a zeolite catalyst generated a CFP oil with the same oxygen content as Pt/TiO_2 (17.3 wt%), but the carbon efficiency was lower (28%). The economics, technical risks, and maturity also vary across the different pathways, and the preferred route will be situationally dependent and based on the available infrastructure and intended downstream use for the CFP oil. Pilot-scale CFP has been demonstrated in both in situ and ex situ configurations using γ-Al_2O_3 (99, 104) and zeolite catalysts (111), respectively. For example, Dayton and coworkers (104) performed a series of experiments at a nominal feed rate of one ton per day in which the temperature was varied from 433°C to 581°C using a λ-Al_2O_3 catalyst and pine feedstock. The CFP oil yield was inversely correlated with temperature and varied from 40 to 50 gallons per dry ton (12–18% carbon efficiency), with oxygen contents ranging 21–31 wt%. Pilot-scale CFP campaigns have also been performed at VTT in Finland. These experiments were performed at 20 kg/h and 520°C with a HZSM-5 catalyst under inert conditions to generate CFP oils with an oxygen content of 21.5 wt% and carbon efficiency of 24% (111). Several commercialization attempts have been made, as highlighted in the sidebar titled Progress in CFP Commercialization.

2.3.3. Research needs. One of the main challenges for CFP is associated with lower-than-desired carbon efficiency. Carbon loss to coke, light gasses, and $<C_5$ volatile compounds reduces bio-oil yields, and the broad product slate results in an inherently nonselective process (81) (**Figure 5*d***). To overcome these issues, integrated catalyst and process development is needed to reduce carbon losses and improve selectivity toward target products. Research activities should also include exploration of alternative reactor designs and heating methods to reduce energy demands and improve efficiency (112). In parallel, strategies must be developed to effectively use byproduct streams (e.g., coke, aqueous, light gasses) to achieve a sustainable and economically viable process (3). Another technical challenge for CFP is associated with inorganic impurities in the biomass feedstocks, such as alkali and alkaline earth metals, which can result in irreversible catalyst deactivation even at low concentrations (113). To address this risk, additional research is needed to establish catalyst tolerance ranges and inform feedstock preprocessing requirements.

PROGRESS IN CFP COMMERCIALIZATION

In 2012, KiOR Inc. attempted to commercialize catalytic fast pyrolysis (CFP) using a zeolite catalyst in a riser reactor. This led to the construction of a commercial-scale facility with a nominal capacity of 500 dry tons per day. This system was operated for approximately 2 years before the company declared bankruptcy in 2014 (81). More recently, Anellotech has completed six months of continuous operation of their TCat-8 facility in Texas and reported process yields of 22–24 wt%. The Anellotech Bio-TCat™ technology, which was originally developed by the Huber group at the University of Massachusetts–Amherst, is a fluid catalytic process for the conversion of nonfood biomass, such as loblolly pine, into benzene, toluene, and xylene (203). Likewise, the Dutch company BioBTX has secured more than €80 million to launch its first commercial-scale plant in the Netherlands, focused on producing sustainable aromatics from plastic waste and biomass using an ex situ CFP process with a zeolite catalyst (204). The increased interest in development of circular materials and biogenic intermediates for refinery integration is expected to support further growth in this technology area.

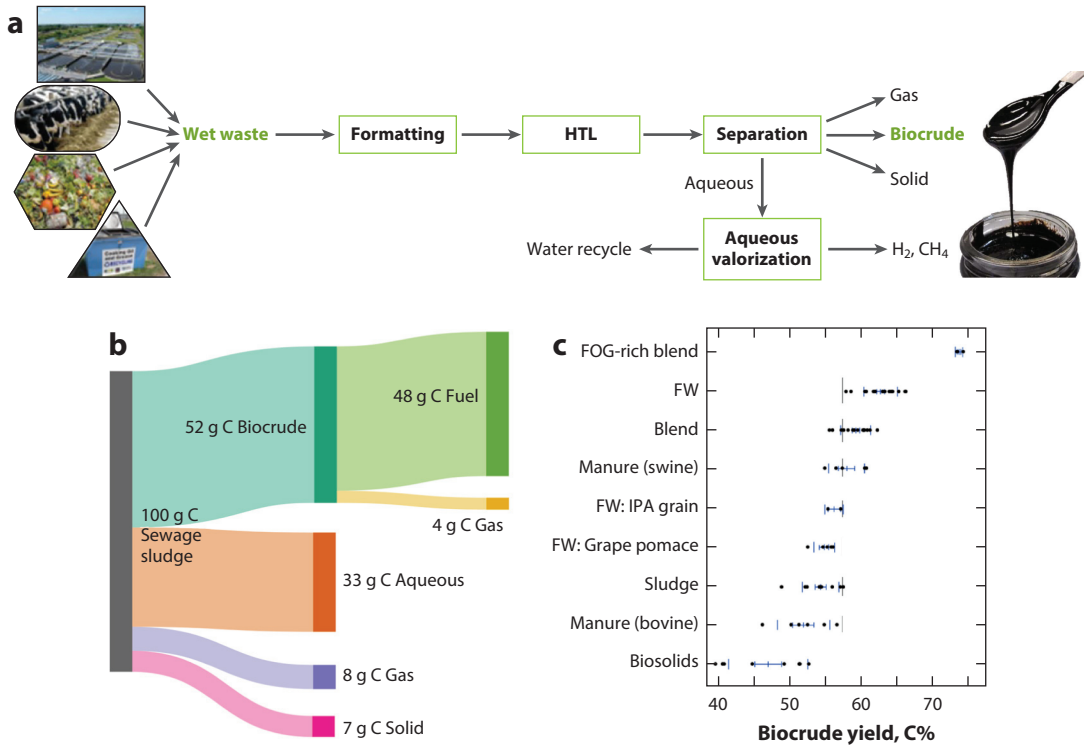


Figure 6

HTL converts wet wastes to biocrude. (*a*) A simplified scheme of the HTL process (formatting includes size reduction, homogenization, and water content adjustment). (*b*) Carbon-based HTL product distribution from a typical sewage sludge (based on data in Reference 118). (*c*) Average product yields (C%) obtained for different types of HTL feed (adapted with permission from Reference 124). Abbreviations: FOG, fat, oil, and grease; FW, fermentation waste; HTL, hydrothermal liquefaction; IPA, India pale ale.

More broadly, accelerated aging protocols are needed to better identify long-term deactivation mechanisms and identify appropriate mitigation strategies.

2.4. Hydrothermal Liquefaction

Hydrothermal liquefaction (HTL) is fundamentally straightforward. It uses water at a moderate temperature (300–350°C) and high pressure (~20 MPa) to liquefy various organic materials into a liquid intermediate known as HTL biocrude (114–117). As a water-based process, HTL is well-suited for feedstocks such as animal manure, wastewater sludge, and food waste, often eliminating the need for energy-intensive drying. HTL produces biocrude, which is thermally stable with a high C content (~70–80 wt%) and a dry higher heating value (~35–40 MJ kg^{-1}) close to that of crude oil (42–47 MJ kg^{-1}), along with aqueous, gas, and solid streams (117, 118) (**Figure 6*a***). Biocrude can be upgraded to fuel-range hydrocarbons via hydroprocessing with high carbon efficiency (>90%; see Section 2.5) (119, 120). Catalysts can enhance biomass liquefaction processes, mainly using homogeneous catalysts such as alkali metals, alkaline earth metals, transition metal salts, and acids (121, 122), with notable efforts also directed toward using heterogeneous catalysts such as transition metal oxides and transition metals (123). Because this review focuses on catalytic upgrading, the predominant focus of this section is to address the impact of catalysts on HTL processes.

2.4.1. Fundamental chemistry. At typical HTL conditions, water stays subcritical and acts as a reactive medium that facilitates chemical bond breakdown and cleavage (115).[6] Subcritical water's permittivity and ionic state shift enhance nonpolar compound solubility and accelerate acid–base-catalyzed reactions like hydrolysis (125). HTL reactions mainly involve the depolymerization of biomass via hydrolysis; degradation of intermediates through dehydration, dehydrogenation, decarboxylation, deoxygenation, and deamination; and rearrangement of resultant reactive compounds through condensation, cyclization, and polymerization. Various homogeneous and heterogeneous catalysts have been used to accelerate these reactions, enhancing biocrude yield and quality simultaneously. The mechanism of catalyst effects still requires better understanding and can be controversial in the literature. The role of catalyst is believed to range from enhancing hydrolysis of polymeric components in feedstock to promoting C–C bond rearrangement and oxygen elimination by acid base functionalities and generating active hydrogen and catalyzing hydrogenation and HDO reactions by metal functions (121–123). These catalysts normally have been used at typical subcritical water HTL conditions.

2.4.2. State-of-the-art comparison. A broad range of feedstocks, such as lignocellulosic biomass, algae, sewage sludge, manure, food waste, and their combinations, have been tested for HTL (124), and the entire process of converting feedstock into hydrocarbon fuels through HTL and hydroprocessing has been demonstrated. **Figure 6*b*** shows a carbon efficiency from sewage sludge to fuel through a typical HTL process (118). **Figure 6*c*** summarizes the biocrude carbon yield from 13 different wet-waste feedstocks (124). Most of the HTL studies use batch systems with scalability constraints, whereas most of the more desired continuous flow HTL systems are limited to lab scale, with some engineering and pilot-scale setups. Demonstration-scale HTL systems for wastewater sludge or woody feedstocks have been announced recently (126). However, the use of catalysts for HTL has been studied largely at lab scale using batch systems with a specific focus on the HTL reaction (123). For heterogeneous catalysts, which are desired from a reusability standpoint, metal oxide–based materials with acid–base functionalities (e.g., CeO_2, ZnO, MgO, NiO, Al_2O_3, La_2O_3, and zeolites), reduced metal or metal sulfides with metallic functions (e.g., supported Ni, Pt, Pd, Co-MoO_x), and their combinations have been demonstrated with advantages in biocrude yield and quality (123). For example, employing a Co-Mg/ZSM-5 catalyst increased the biocrude yield from ~40% to ~60% for the HTL of food waste using a batch reactor (127). Supported CoMo catalysts enhanced the biocrude yield, reduced its oxygen content, and increased the higher heating value of biocrude in the HTL of a sewage sludge using a micro-batch reactor (128).

2.4.3. Research needs. One of the major challenges for the commercial implementation of HTL is practical operability, primarily due to reactor fouling, which impacts heat efficiency and continuous flow operation. At elevated temperatures, biological materials undergo various morphological changes to form solid precipitates, whereas inorganic minerals can form precipitated salts. Furthermore, the high viscosity of the slurry feeds results in poor heat transport properties and significant temperature gradients near heat transfer surfaces, promoting fouling and necessitating large, capital-intensive heat exchangers. New reactor designs are therefore required, along with a better understanding of the complex reactions and kinetics in HTL of real-world feedstocks and improved strategies for using or recycling aqueous and solid coproducts of HTL. In particular, the application of catalysts in the HTL process to reduce reaction severity

[6]The altered permittivity and density of subcritical water make it less polar, thereby enhancing the solubility of nonpolar compounds.

and costs while increasing bio-crude yield and quality is attractive. However, there is a need to better understand the mechanism of catalytic reactions, identify heterogeneous catalysts for these desired chemistries, demonstrate the advantage of catalysts in continuous flow HTL systems, and address issues around catalyst longevity and/or recovery.

2.5. Hydroprocessing

Catalytic hydroprocessing is one of the most widely used unit operations in petroleum refining, with a capacity of >19 billion barrels per day in the United States in 2023 (129). Similar processes can be applied to biomass- and waste-derived liquid intermediates to produce biofuels or fuel blendstocks, with key reactions removing heteroatoms and increasing energy density to meet fuel specifications (130–132). This section concentrates on the hydroprocessing of emerging bio-intermediates and does not cover established pathways such as hydrotreating esters and fatty acids. Many bio-intermediates are highly reactive due to carbohydrate-derived components such as aldehydes and anhydrosugars (133–135) or lignin-derived compounds with conjugated double bonds (136). This can lead to hydroprocessing catalyst deactivation and reactor fouling and necessitate reducing the concentration of these compounds prior to hydroprocessing. Many hydrotreating feedstocks may be acidic and incompatible with reactor metallurgy, and/or may require the removal of impurities (137), such as metals, which negatively impact hydroprocessing catalyst activity (138). Hydroprocessing of bio-intermediates is accomplished either via co-processing with petroleum streams in existing refineries or as standalone processes in dedicated biorefineries. Co-processing in refineries offers a cost-effective solution but brings uncertainty to current refinery operations (138).

2.5.1. Fundamental chemistry. The hydroprocessing reactions (**Figure 7*a***) include reactions to remove heteroatoms [HDO, hydrodesulfurization (HDS), and hydrodenitrogenation (HDN)], improve fuel quality (hydrogenation and hydroisomerization), and convert heavy hydrocarbons into lighter, more desirable products (hydrocracking). HDO is necessary for all bio-intermediates, though some feeds, e.g., HTL biocrude from food waste or sewage sludge, have high nitrogen contents requiring extensive HDN. A competition between the hydroprocessing reactions and polymerization of the reactive components requires careful selection of operating conditions and often pretreatment to produce a more stable bio-intermediate (139). HDO reactions may compete with other reactions, e.g., HDS or HDN, for the same catalyst active sites, which can be problematic for co-hydroprocessing. Traditional supported CoMo- and NiMo-based sulfides are the main catalysts evaluated for upgrading biomass-derived streams (95, 107, 120). In addition, noble metals (e.g., Ru, Pd, and Pt), base metals (e.g., Ni), and metal phosphides and carbides have been studied, mostly for HDO and hydrogenation of model compounds and stabilization of the bio-intermediates.[7]

2.5.2. State-of-the-art comparison. Bio-intermediate quality impacts the hydrotreating process and the product properties. Many feedstocks, e.g., pyrolysis bio-oil, require stabilization prior to hydroprocessing. CFP oil hydrotreating has been demonstrated for hundreds of hours of time on stream (146, 147). Sulfided NiMo and CoMo (95, 107, 140) give good HDO performance but require high temperatures (~400°C) and pressures (>100 bar) and low space velocities (0.2 h^{-1}). Other catalysts have not been tested in continuous systems but appear to require similar pressures (>100 bar) and temperatures (≥350°C) (148–150). Alternative bio-intermediates, e.g., HTL

[7] Stabilization prior to hydroprocessing can include methods for hydrogenating reactive carbonyl and phenols or processes such as catalytic fast pyrolysis (see Section 2.3).

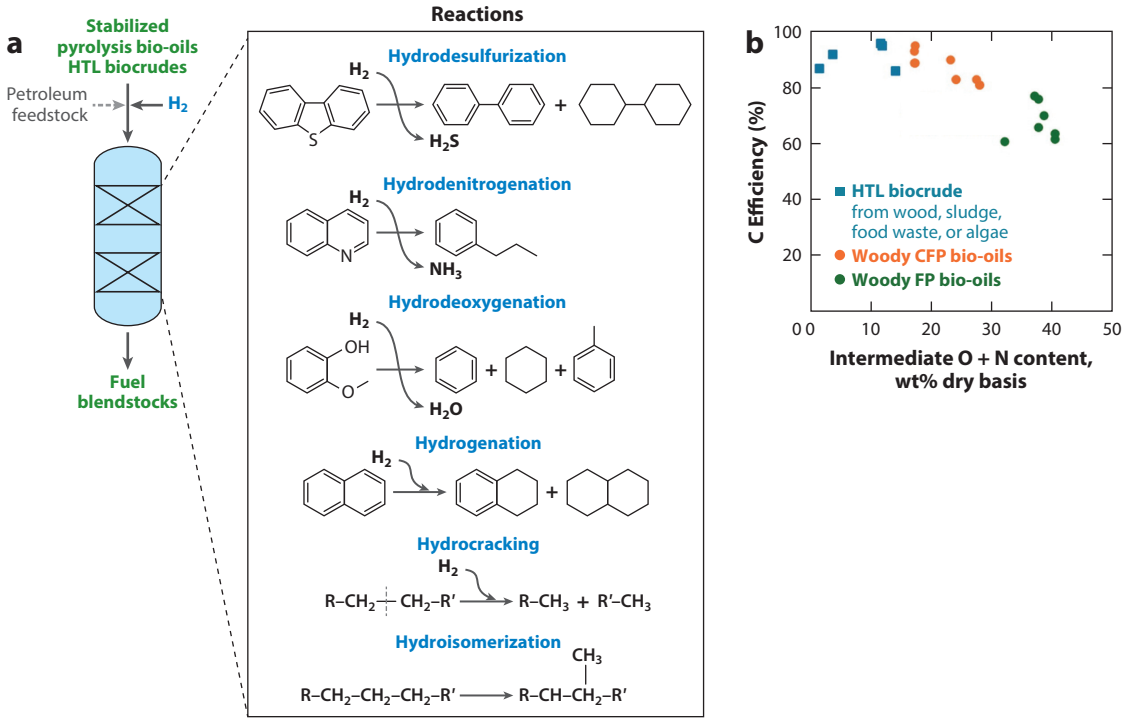


Figure 7

Hydrotreating of biomass- and waste-derived liquid intermediates (pyrolysis bio-oils and HTL biocrudes): (*a*) Key hydroprocessing reactions involved for heteroatom removal and fuel quality/yield increase. (*b*) Hydrotreating carbon efficiency dependence on heteroatom (O and N) content in liquid intermediates estimated from References 95, 105, 120, 140–145 for HTL biocrude from sludge, food waste, and algae (N content is included). Abbreviations: CFP, catalytic fast pyrolysis; HTL, hydrothermal liquefaction.

biocrudes, can be hydroprocessed without stabilization (119, 120, 151), and more than 1,500 h of time-on-stream has been demonstrated for them.

Hydrotreating carbon efficiency decreases with increasing bio-intermediate oxygen content: e.g., non-CFP with ~40% oxygen, CFP oils with 15–25% oxygen, and HTL biocrudes with ~5% oxygen give carbon efficiencies of 60–80%, >90%, and >95%, respectively (**Figure 7*b***). The fuel quality varies. Adding a hydrogenation zone before final hydroprocessing improved the cetane number of the diesel product (141) from CFP oil and produced fractions with promising aviation fuel properties (96), though this approach further decreased the space velocity. Hydrotreating HTL oil from wet waste produced a diesel-rich fuel blendstock with a high cetane number due to the high fraction of alkanes (120). The jet fraction exhibited key fuel properties within the required range for aviation fuel (151).

Co-hydroprocessing CFP oil or HTL biocrude with petroleum streams such as vacuum gas oils and straight-run diesel at blend levels of up to 20% gave a near-complete upgrading (HDO or HDS) at less severe conditions compared to standalone hydrotreating. The biogenic carbon yield in co-processed fuel products aligned with or exceeded the standalone carbon efficiency.

2.5.3. Research needs. Despite significant advancements, catalyst deactivation and reactor fouling and plugging during extended operation remain major challenges for hydroprocessing of bio-intermediates. The level of stabilization or contaminant removal needed before

hydroprocessing must be defined and the key material attributes and their tolerance limits identified. Understanding catalyst deactivation mechanisms is essential for developing strategies to mitigate deactivation and fouling. Extended continuous operation for thousands of hours needs to be achieved, and the process needs to be scaled up to produce sufficient quantities for comprehensive fuel property analysis and engine testing. Strategies should be developed to increase fuel quality and the fraction of desired fuel cuts, e.g., aviation fuel, by enhancing the coupling of gasoline-range molecules and cracking of heavier cuts.

3. ENABLING CAPABILITES FOR CATALYST DEVELOPMENT

3.1. Advanced Synthesis

Advances in catalysts for biomass upgrading reactions require control across multiple scales: atomic-scale control over multifunctional active sites (e.g., H_2-activating, acidic, basic), followed by micro- and meso-structural control for product shape selectivity and mass transport. These complex requirements are driven by a diverse slate of reactions inherent to biomass upgrading, as well as considerations for industrial operation. The synthesis of supported heterogeneous catalysts has been widely studied (152–154). However, the complexity of these systems requires new approaches to accelerate the process of catalyst discovery and development, especially for emerging biomass conversion processes. Here, we discuss two such approaches, one focused on active site control through continuous flow synthesis and another targeting the transition of research catalysts to engineered catalyst forms. Both rely on rapid feedback between catalyst synthesis and characterization to accelerate catalyst development.

3.1.1. Continuous flow synthesis as a platform for catalyst discovery. The synthesis of supported materials for heterogeneous catalysis has been widely studied, and several methods have been commercially deployed, including coprecipitation and impregnation. Some adaptations of these approaches (e.g., strong electrostatic adsorption) have been used to prepare single-atom catalysts or nanostructured active phases with narrow size distributions, targeted compositions, or well-defined surface structures (152–154). However, adaptations of wet impregnation and coprecipitation routes have their limitations in asserting morphological and compositional control and, additionally, are extremely sensitive to the support material. This support dependence prevents the developed structural control schemes from being generalizable and limits their relevance to a small subset of materials. Despite these limitations, these techniques remain ubiquitous in industrial catalysis due to their ease of operation, scalability, and low cost, but several new synthetic methodologies on the horizon promise the operability and throughput of traditional methods while affording precise morphological/compositional control and being support agnostic.

One example encompasses micro- and millifluidic reactor technologies, which have emerged as platforms for the continuous flow synthesis of solid catalysts that overcome limitations inherent in batch solution-phase reactions (155, 156). The small fluid channel dimensions promote rapid heat and mass transfer, increase yield and throughput, and enable parallel scaling. This process-intensified approach has been applied for the synthesis of metal and metal oxide nanoparticles, supported metal atoms and particles, zeolites, and metal-organic frameworks, among others that are relevant for biomass catalysis (155). Further, these continuous flow reactors can be used to rapidly screen reaction conditions (e.g., temperature, residence time), which makes them suitable for integration with state-of-the-art data-driven techniques for multivariate materials and process optimization, ultimately enabling acceleration of catalyst development (157). Statistics-based regression techniques such as design of experiments and response surface methodology can be applied to map synthesis reaction conditions (inputs) to outcomes (responses) that are continuous in nature (e.g., particle size, yield). Machine learning (ML) approaches such as Bayesian optimization

can be used for complex systems and categorical or discrete outcomes (e.g., crystalline phase) (158). For example, ML algorithms have been used successfully to quantitatively determine the effects of crystallization conditions on the microstructural characteristics of a faujasite zeolite. This has led to improved catalytic properties, demonstrating the impact these approaches can have on controlling complex catalysts that are relevant for biomass conversion processes (159). Determining the outcomes of these experimental screenings, however, requires ex situ characterization, which becomes a bottleneck in the iterative optimizations. Alternatively, in situ characterization by UV-visible spectroscopy, X-ray absorption spectroscopy, or small-angle X-ray scattering, for example, can provide real-time information at different points in time and space during the continuous flow synthesis of catalyst materials, enabling a wide parameter space to be swept in a single experiment (155).

3.1.2. Transitioning from research catalysts to engineered forms. However, discovery is merely the first step along the journey toward commercial deployment and real-world impact for a catalytic material. Transitioning the highest-performing catalysts from the laboratory to an industrially relevant environment bears its own set of unique challenges, both technical and economic. Fundamentally, this begins with the translation of a relatively simple powdered research catalyst (i.e., active phase and support) to an industrially relevant engineered catalyst [i.e., multicomponent shaped technical body (160, 161)]. Consequently, preparation of these macroscopic forms (i.e., micrometer to centimeter diameters) often requires additional components to engender the desired operational performance (e.g., minimize pressure drop, mechanical strength), which alters their composition, structure, and porosity relative to their powdered counterparts. These changes can significantly impact catalytic performance, yet little information is available in the open literature regarding the form–function–performance relationships of these complex technical bodies. Therefore, small-scale manufacturing methods accessible at the laboratory scale, rapid multiscale characterization techniques, and high-throughput catalytic evaluation, coupled with data-driven analysis, are needed to navigate the nonlinear transition from research to engineered catalyst (162). Catalytic testing of engineered materials, for example, requires reactors of sufficient scale with appropriate kinetic and mass transport and hydrodynamic parameters for the millimeter-scale catalysts, as well as correspondingly high reactant delivery. In contrast, approaches for evaluating catalysts using only a single or a few particles are more amenable to a laboratory research environment and enable higher-throughput evaluation. Data collected from these evaluations can be directly incorporated into computational fluid dynamics (CFD) simulations to provide feedback on catalyst properties, enabling rapid, iterative development of engineered catalysts.

3.2. Advanced Characterization

Advancement of biomass conversion catalysts requires an understanding of catalyst evolution under working conditions and transitioning critical catalyst active structures to formed materials for industrial scale-up. In this section, several impactful, state-of-the-art characterization techniques are discussed for understanding catalyst deactivation and emerging techniques for comprehensively analyzing engineered catalyst forms.

3.2.1. Characterization of catalyst deactivation. Catalyst deactivation in biomass upgrading is often distinguished by decomposition of reactive hydrocarbons and oxygenates to graphitized species (coke) (81, 163, 164), or sintering/clustering of active metal sites under the demanding reaction conditions required (165–167). Although many analytical techniques have been employed to monitor catalyst structural changes both in situ and postmortem, here focus is placed on a single technique that has been particularly impactful for the characterization of spent and working biomass catalysts. Confocal fluorescence microscopy (CFM) is a valuable analytical tool for

monitoring the formation and spatial distribution (at nanometer scale) of organic species deposited during reaction due to their fluorescent properties (164, 168–170). This technique is of particular relevance to biomass conversion catalysts, including predominantly zeolite-based materials, because the nature and location of carbon deposition strongly depend on the reactant molecule, the strength and accessibility of acid sites, and the properties of dopant or binder materials (163, 164, 168, 171). In the etherification of glycerol with various alkenes over H-beta zeolite, Heracleous et al. (164) characterized increasing coke accumulation on the outer shell of zeolite crystallites with increasing alkene chain length (C_8–C_{12}) by CFM measurements. The results could be related directly to reduced activity with increasing zeolite crystallite size (average diameter: 0.1 to 9.0 μm) due to the increasing accessibility of external surface sites (164). When combined with other atomic to microscale characterization techniques, such as X-ray (micro/nano)tomography, photoelectron X-ray spectroscopy, tip-enhanced fluorescence microscopy, (operando) scanning transmission electron microscopy, small-angle X-ray scattering, or atom probe tomography (172, 173), CFM can provide comprehensive insight into deposited carbon at various lengths and timescales of catalyst deactivation.

3.2.2. Characterization of engineered catalysts coupled with machine learning. The transition from a powder research catalyst to a formed engineered catalyst introduces increased complexity (e.g., mesoporosity, binders with different composition, inhomogeneities from preparation) across disparate length scales, necessitating the use of diverse characterization techniques to establish a comprehensive understanding of the engineered catalyst system (174, 175). Extruded catalysts, for example, require multiscale (mm-μm-Å) characterization to account for structural heterogeneity across all relevant length scales to fully understand their properties and performance and how they tie back to the synthesis approach (structure–property–synthesis–processing). X-ray computed tomography (XCT), currently deeply applied in additive manufacturing research, can characterize microporosity and provide 3D information on the catalyst mesostructure. As an example, Owen et al. (176) used nano-XCT to understand the degradation of supported Ni/Co catalyst particles during CO_2 reforming of methane due to catalyst breakdown and coke formation (**Figure 8**). Specifically, XCT creates an opportunity to capture information throughout the large volume of the material on morphology (e.g., porosity, cracks), phases, and material degradation causing performance decay. Results from such can be applied for improving calculations on transport properties and the multiscale computational modeling study of biomass fast pyrolysis (177). In

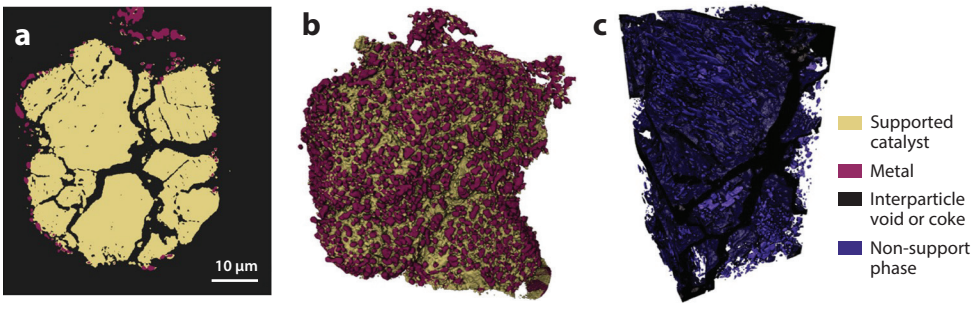


Figure 8

X-ray nano-computed tomography of spent Ni/Co/Al_2O_3 CO_2 reforming catalyst showing (*a*) segmented ortho-slices, (*b*) full sample volume rendering, and (*c*) internal non-support phase volume rendering (yellow, supported catalyst; purple, metal; black, interparticle void or coke; blue, non-support phase). Figure reproduced from Reference 176 (CC BY 4.0).

addition to the increasing complexity of the catalyst material, data collection from these techniques is no longer rate-limiting, as novel high-throughput and operando experiments yield increasingly large and complex data sets. Consequently, data-driven tools are being developed to accelerate the analysis of spatially distributed data and coupled spectroscopic information to uncover connections between catalyst structure and performance. For example, a deep-learning method has been established for the automated detection of metal centers in high-resolution scanning transmission electron microscopy images of single-atom catalysts based on difficult-to-image carbon-type materials (178). One area of growth is the movement from 3D to 4D catalysis, where advances in experimental tools and computation are needed to understand dynamic catalyst behaviors through time-resolved operando characterization (179).[8]

3.2.3. Future opportunities. Accelerating the catalyst development timeline requires valuable feedback from cutting-edge characterization tools. Enhanced understanding of the working state, deactivation pathways, and regenerability of the catalyst through such techniques and expanding this to scaled-up, engineered particle forms will be essential to continued material advancement. In this respect, as catalysts become increasingly complex, integration of artificial intelligence into characterization workflows can increase both productivity and processes for standardization in data analysis among researchers for improved biomass catalyst process development.

3.3. Multiscale Modeling

Combining theoretical and experimental approaches allows for a more robust fundamental science basis for enabling rapid advancement of bioenergy technologies. In the acceleration of catalysis science for bioenergy solutions, computational science can provide useful predictive surface structures to accelerate catalyst discovery and means to predict catalyst performance in scaled-up systems and processes. We give examples of both below.

3.3.1. Deoxygenation of bioenergy intermediates. One example for which computational science methods have been critical to biomass catalysis research is in the catalytic upgrading of bio-intermediates, specifically in understanding deoxygenation mechanisms key to chemical utilization. Density functional theory (DFT) allows precise calculation of atomic-scale catalysis reactions on specific material surface structures and is a primary method for understanding deoxygenation. You et al. (180) applied DFT to evaluate Cu/Mo_2C catalysts to HDO of 1,2- and 1,3-propanediols to evaluate the role of hydrogen and O–H bond scission reaction steps in the catalytic process. The phenomena modeled by DFT can often be observed with spectroscopic and characterization techniques, which allows for improved overall understanding and verification of the processes. Murphy et al. (181) showed the benefits of combining modeling with characterization experiments for a similar class of Mo_2C as well as other catalyst materials. The authors provided an excellent example of the benefits of combining computational and experimental techniques to further understand the catalysis and discussed the connection to reaction kinetics and challenges with applications to realistic process environments. Ren et al. (182) also combined characterization and DFT modeling for catalytic HDO with Mo_2C catalysts; their characterization includes detailed structural information obtained via X-ray diffraction and electron microscopies. Here DFT has proven to be valuable in determining the relative selectivity of catalytic scission of C–O, C=O, and C–C bonds, which is critical to deoxygenation while preserving molecules suitable for fuel. Ignatchenko (183) explored DFT as applied to ketone production from carboxylic acids.

[8]Transition from 3D to 4D catalysis involves cross-coupled characterization of catalytic centers (3D) over dynamic time scales (+1D).

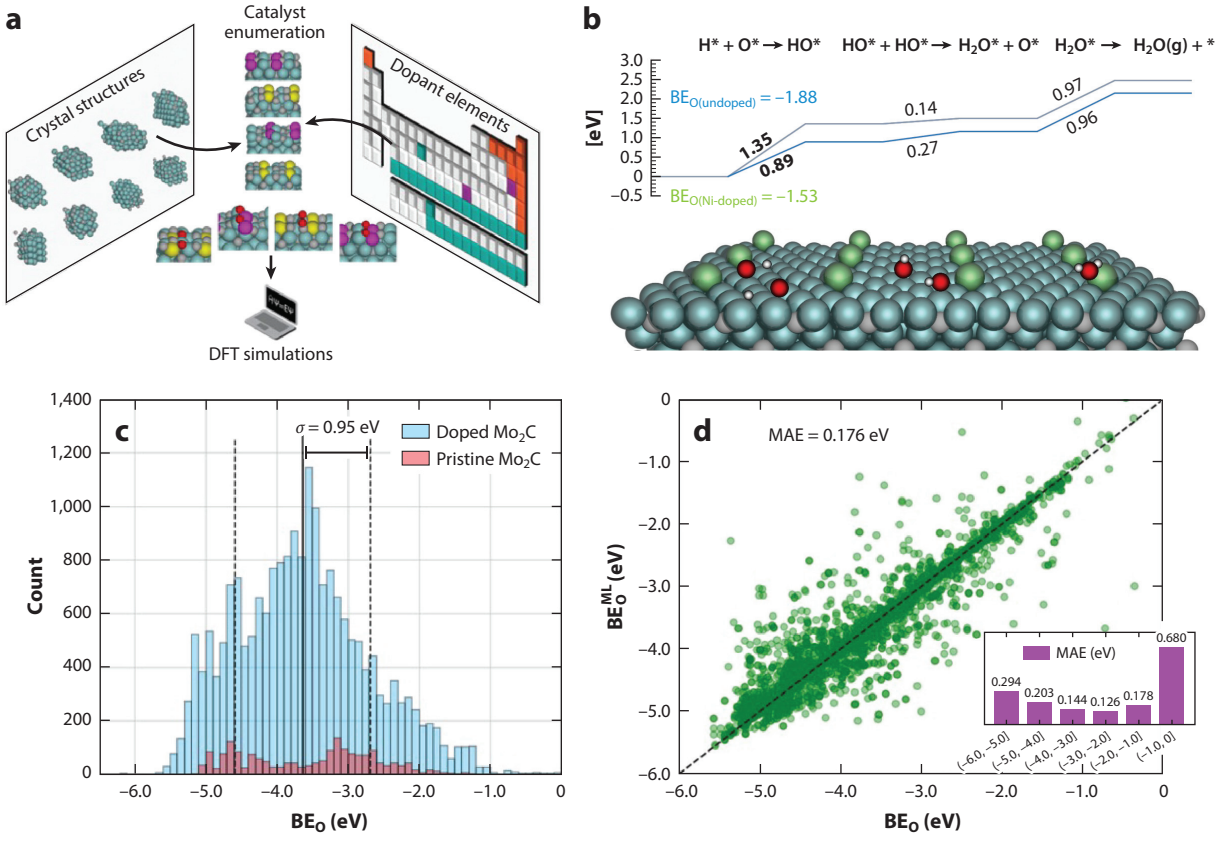


Figure 9

(*a*) High-throughput structure enumeration and first principles–based data generation for oxygen adsorption on pristine and doped Mo_2C catalyst surfaces. (*b*) DFT-computed stepwise thermodynamic energy profile for deoxygenation of spent nickel-doped Mo_2C catalyst surface. (*c*) DFT-computed oxygen binding energy distribution on pristine and doped Mo_2C facets. (*d*) Parity plot of oxygen binding energies predicted by our deep-learning graph neural network, LCG-MPNN (BE_ML), and computed by DFT (BE_DFT). Abbreviations: DFT, density functional theory; MAE, mean absolute error. Figures are reproduced from Reference 185 (CC BY 3.0).

Jiao et al. (184) used DFT combined with multiple spectroscopic and characterization methods to study the role of K-modified catalysts for catalytic CO_2 gasification of sawdust char.

Use of high-performance computing (HPC) coupled with DFT calculations enables a greater range of catalytic material combinations to be evaluated and assessed for optimization. Doan et al. (185) explored 20,000 variations of Mo_2C-dopant combinations via DFT on HPC, and ML algorithms have been applied to the resulting data set for oxygen binding energy prediction. **Figure 9** describes their process. The combined advancements in computing throughput and ML provide emerging opportunities for greater use of DFT for catalysis discovery and understanding for bioenergy applications.

3.3.2. Reaction kinetics and role in reactor modeling. Although catalytic mechanisms occurring at material surfaces are captured with DFT modeling, simulating catalyst performance requires an understanding of reaction kinetics under operating conditions. Deoxygenation is also a focus of process- and reactor-scale research; Tirado et al. (186) reviewed catalysts and kinetic modeling for the hydrotreatment of bio-oils. Their work includes the application of kinetics to

reactor models, which is critical to enabling scale-up of bioenergy catalysis processes. Goyal et al. (187) show the complexity of catalyst particle effects in catalytic upgrading reactors; the application is for upgrading of pyrolysis vapors. Here, due to the complexity of the chemistry, a common lumped form of kinetics is applied as a simplifying assumption. Nonetheless, the work describes important phenomena occurring in a catalytic riser reactor via both detailed CFD and reduced-order reactor modeling. Due to the variety of pathways for converting biomass into fuels and chemicals, computational modeling has been applied in a wide range of applications and reactor systems. Specifically, Lasich (188) applied modeling to a process using a pressure swing adsorption reactor and bentonite clay catalysts for the conversion of wood gas upgrading.

Similar to the case for DFT modeling for catalysis research, HPC capabilities are also advancing reactor modeling potential. Performing models with CFD is computationally intensive, and as reactors scale, the computational resources needed scale as well. However, new advancements in CFD codes are enabling a new paradigm in reactor modeling. Musser and colleagues (189, 190) have developed an exascale version of the open-source Multiphase Flow with Interphase eXchanges (MFiX) that is being used to perform CFD on the most advanced HPC systems, including exascale computers. These new advancements will enable a broader range of reactor designs to be studied and greater resolution for commercial-scale reactors.

3.3.3. Future opportunities. Although the application of computational modeling to bioenergy challenges has proven advantageous, especially when coupled with complementary experimental techniques, the complexity of bioenergy chemistry and the need to scale bioenergy processes up effectively represent major challenges moving forward. To address these challenges, approaches that connect atomic-scale catalytic phenomena to realistic processes and reactor scales are needed. Deshpande & Vlachos (191) demonstrated DFT as applied to complex atomic surface structures coupled with X-ray adsorption spectroscopies as next-generation model-experiment approaches to understand complex catalysis. Šivec et al. (192) reviewed multiscale modeling approaches for the conversion of furfurals and levulinic acid from hydrolysis of furans that encompasses atomic-scale mechanisms, microkinetics, and additional techniques toward comprehensive reactor models. These approaches, while challenging, represent the necessary tools required to connect reactions at the fundamental science level to complex engineered systems at scale. Fortunately, computer speeds and related computational methods are advancing rapidly to enable multiscale approaches. In addition, the computational science advancements are enabling the application of advanced techniques such as artificial intelligence and ML that, when supplied with sufficient data and modeling results, can further accelerate catalyst discoveries. Jin et al. (193) demonstrated the application of neural networks to biodiesel as a method that benefits from advancing computational capabilities.

4. OUTLOOK

As is hopefully clear, the challenges the catalysis research community faces in meaningfully impacting planetary-scale processes of energy and materials production require a departure from business as usual. The extraordinary time frame in which technologies must be discovered, derisked, and deployed necessitates complementary research in methods, frameworks, and tools that accelerate the entire process. One obvious (and yet unrealized) opportunity is the development of discovery tools that can rapidly identify high-performance materials for converting disparate biomass resources into fuels and chemicals that circumvent time-consuming Edisonian down-selects and surveys.

The rational design of high-performance catalysts for a targeted transformation has long been one of the holy grails of heterogeneous catalysis. To date, most attempts at rational design have

relied on a concerted experimental and computational approach to elucidate key performance descriptors and inform catalyst selection (194). In general, this strategy has been most successful when considering relatively idealized systems (e.g., periodic surfaces, static particle morphologies, well-defined interfaces and faceting) and demonstrated using relatively simple chemical transformations (or a small set of adsorbates) due to the time-intensive nature of DFT. This limits the parameter space that can be reasonably explored in most research settings. However, the complexities of catalyst synthesis (i.e., nontrivial production of targeted properties), catalyst operations (i.e., catalyst evolution/deactivation/poisoning during reaction), and bioenergy-related feeds (e.g., biomass vapors, bio-oils) further divorce predicted performance and reality. Further, these complexities consider only powdered research catalysts. Translation to a more commercially relevant engineered catalyst presents a host of disparate concerns, including economics, feasibility, and safety of manufacture and scale-up, as well as maintaining performance and durability when introducing non-innocent structural agents to impart required mechanical properties.

To address these challenges, several computational/experimental workflows have been designed (like those described above in the multiscale modeling section), which has resulted in the development of a handful of supporting tools and databases to aid in catalyst design. With the emergence of powerful ML implementations in catalysis (195–197), one of the most critical needs to apply these capabilities to the design of catalyst materials for bioenergy applications is access to high-quality experimental and computational data sets for training ML models. In recent years, several databases have emerged to fill this research gap, focusing on computational data [e.g., Open Catalyst Project (195) and Catalysis Hub (198)], experimental data [e.g., CatTestHub (199, 200)], or the interface of both [e.g., Department of Energy Data Hubs (201, 202)]. These data platforms have manifested several approaches to maintenance and growth, with some using a crowd-sourcing approach to seek data from contributors, hosting of member-organization generated data, or curation of peer-reviewed sources. However, in general, there is limited availability of data related to bioenergy applications (i.e., large biomolecule-derived adsorbates) published therein. In addition, catalyst design demonstrations that have leveraged either ML approaches or combined computational/experimental workflows have done so using bespoke tools and not a general framework or product.

These databases represent the shared expertise and resources of several collaborative bodies that seek to advance the state of the art in energy materials research. However, no comprehensive tool or suite of tools exists that covers the diversity of research challenges associated with catalyst design for bioenergy applications. Integrating the elements described above with nascent ML technologies and large, high-quality databases of experimental and computational data could dramatically reduce the time from novel synthesis to commercial implementation for the bioenergy technologies of the future.

SUMMARY POINTS

1. Thermal catalytic processing of biomass feedstocks and derivatives to valuable fuels and chemicals offers an opportunity to increase domestic energy production. Nevertheless, catalyst development in this area is inherently complex given the multifaceted nature of biomass feedstocks and the associated conversion technologies.
2. In the catalytic upgrading of biochemical intermediates, a diverse range of materials can be produced, each presenting unique challenges from a chemical conversion perspective. In the case of alcohols, acids, and furans, current research commonly reflects the need

for developing multifunctional catalysts that can reduce the number of upgrading unit operations, with a focus on engineered catalyst materials which show resistance to long-term deactivation pathways.

3. Translating the capabilities of powder, lab-scale catalysts to engineered forms for large-scale operation is critical to the development of many of the identified bio-conversion processes. As presented in analogy to industrial methanol-to-hydrocarbon reactions, key issues including appropriate mechanistic studies, reactor selection, process demonstration, and catalyst regeneration strategies present major hurdles to process development, even in the case of more basic feedstocks, such as syngas and C1 oxygenates.
4. Understanding and mitigation of catalyst deactivation through coking is a common hurdle among the identified catalytic processes. As in CFP, the formation of unwanted coke also leads to reduced carbon efficiency of the process, one of the main challenges. Inorganic impurities present in the biomass feedstock can further result in irreversible catalyst deactivation.
5. During hydrothermal liquification and catalytic hydroprocessing applications, upgrading of the biomass intermediates can cause significant reactor fouling and plugging during extended operations, leading to recurrent shutdowns. Future developments in reactor optimization and mitigating catalyst deactivation mechanisms will be essential to meeting requirements for extended, continuous reactor operations.
6. Nascent and state-of-the-art technologies progressing catalyst synthesis and characterization offer multifaceted approaches toward formulating and understanding the properties of engineered and large-scale produced catalyst materials. Unlike traditional lab-scale powder catalysts, capabilities are needed to optimize and characterize several length scales (mm-μm-Å) to enable required developments for commercialization.
7. To accelerate process development, experimental-lead theoretical approaches offer a valuable guide for atomic-scale fundamental insight and rapid technological advancement. Kinetic and reactor modeling can become increasingly complex for associated bioenergy chemistries; however, advancements in computational science (e.g., artificial intelligence and machine learning) may aid in addressing challenges of multiscale catalytic phenomena.

FUTURE ISSUES

1. To enhance the value of bioderived fuels and chemicals, how can multifunctional catalysts be further explored and exploited for biomass conversion technologies? What tools and techniques should be developed to answer these multifaceted, complex challenges?
2. How can catalyst flexibility be promoted to create conversion processes that can adapt to diverse and unconventional bio-feedstocks?
3. As technologies are advanced toward industrial adoption, what challenges will be faced at intermediate and industrial scales? What developments in reactor design and scaled-up catalyst synthesis are needed to meet these demands and reduce technological and financial risks?

4. To capture the complexity of biomass feedstocks, what components of reactor-scale models are required to accurately simulate catalytic and transport phenomena while maintaining computational feasibility? This accuracy is critical to meeting scale-up objectives and design optimization and in considering the commercial viability of a given process.

DISCLOSURE STATEMENT

M.B.G. holds US Patent 11,766,661 B2, "Materials and Methods for Improved Pyrolysis Processing" (2023). D.A.R. received funding to research syngas to hydrocarbons chemistry and holds US patents for methanol and syngas conversion to fuels.

AUTHOR CONTRIBUTIONS

J.N.H. contributed to conceptualization, methodology, writing the original draft and review, and editing. J.H.M. contributed to conceptualization, methodology, data curation, writing of the original draft and review, editing, and visualization. R.S.A., F.G.B., S.E.H., K.I., T.R.K., A.K., J.G.L., A.M., A.S., A.D.S., M.R.T., K.A.U., H.W., A.W., and X.Y. contributed to writing, editing of the original draft, and review. R.D. and V.D. contributed to acquisition of the data, the analysis, the interpretation of the data cited in the manuscript, and writing of the original draft. M.B.G. contributed to conceptual design, analysis, and interpretation of data as well as writing, editing, and reviewing the manuscript. C.M. contributed to formal data analysis, review, and editing. J.E.P. II contributed to the literature review, acquisition of data for the work, writing a section of the original draft including intellectual content, and editing and revising the work. D.A.R. contributed to funding acquisition, writing, and editing of the original draft. J.A.S. contributed to conceptualization, methodology, funding acquisition, reviewing the original draft, and editing.

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