Review

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Review

A Comprehensive Review on Biomass Valorization Through Thermochemical Pathways: Product Properties and Usage of Artificial Intelligence

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Abstract

Biomass valorization plays a vital role in achieving carbon neutrality and circular economy frameworks. Owing to its carbon rich structure, biomass represents a promising feedstock to produce bio-based hydrocarbons via biological and thermochemical pathways. While biological conversion routes have been extensively studied, their deployment at commercial scale is constrained by high capital costs and low product yields. In contrast, thermochemical conversion technologies are increasingly being explored as viable large scale biomass valorization routes. This review presents a comprehensive assessment of thermochemical pathways, with particular emphasis on hydrothermal liquefaction (HTL). HTL enables the efficient conversion of wet and heterogeneous lignocellulosic biomass without energy intensive drying pretreatments. The review critically examines the formation and physicochemical properties of the two main HTL products, namely liquid biocrude and solid hydrochar. Special attention is devoted to challenges associated with biocrude quality, particularly its high oxygen content, and corresponding upgrading strategies. Additionally, the diverse applications of hydrochar for energy recovery, soil amendment, and heterogeneous catalyst synthesis are discussed. The article also compares the technology readiness levels of thermochemical conversion routes and highlights the growing role of artificial intelligence and machine learning in process modelling and optimization. Finally, future research directions are identified, emphasizing design by specification strategies and physics informed AI to enable scalable, autonomous biomass conversion technologies.

Keywords: biomass valorization; hydrothermal liquefication; biocrude upgrading; hydrochar application; artificial intelligence

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1. Introduction

Biomass serves as a versatile resource for industries in animal fooding, textiles, construction, soil improvement, chemicals, and energy sectors. In the global pursuit of sustainability, carbon neutrality, and reduced environmental impact, biomass has emerged as a key contributor to circular economic strategies. Its organic and renewable nature makes it an attractive alternative to fossil-based resources. However, using primary biomass for energy directly competes with food production, which has a higher priority [1]. This challenge highlights the importance of second-generation biofuels, derived from agro-forestry residues, and other waste streams. The biomass waste used for producing second generation biofuels share similar chemical compositions with fossil-based feedstocks. Further, biomass offers advantages such as high abundance, renewability, and biodegradability, which makes them a promising solution for sustainable energy and resource recovery [2]. Organic residues contribute 46% of cumulative global solid wastes, where agricultural, industrial and urban-area produced residues are the chief contributors [3]. Agricultural and forestry operations generate substantial quantities of lignocellulosic residues, including husks, straws, sawdust, and wood shavings. These bio-residues, primarily composed of cellulose, hemicellulose, and lignin, represent the most abundant renewable biomass resource on Earth. Owing to their chemical complexity and structural diversity, lignocellulosic biomass is increasingly recognized as a versatile feedstock for energy and chemical productions. The unique chemistry of its major components enables the development of advanced biorefinery processes, positioning lignocellulosic biomass as a cornerstone for future bio-based industries [4]. Biofuels derived from lignocellulosic biomass are widely regarded as carbon-neutral alternatives to fossil fuels for the transportation and energy sectors. Currently, fossil fuels dominate the global primary energy supply, accounting for approximately 81%, followed by renewable sources at 14% (biomass contributes 70%) and nuclear energy at 5%. The global annual biomass supply from agriculture and forestry is estimated at approximately 12 billion tons of dry matter, with agriculture providing about 61% (47% from crops and 14% from above-ground residues) and forestry contributing the remaining 39%. These figures underscore the vast availability of biomass resources and their critical role in advancing sustainable energy systems [4,5]. Figure 1 illustrates different sources of biomass along with their end-to-end distribution for different applications. The major sectors where the produced biomasses are used differ depending on the source of residue production, like crop residues are chiefly used as animal food and bioenergy synthesis. Whereas bio-based residue produced from wood industry is chiefly used in the energy sector followed by the biomaterials industry [6].

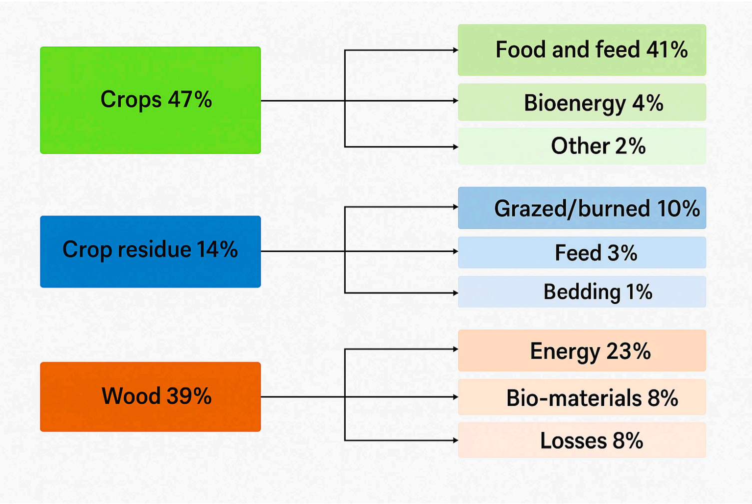

Figure 1. Lignocellulosic biomass sources and end-use distribution.

2. Thermal Conversion of Bio-Based Residues

Vegetal biomass is an abundant, and easy to acquire resources which can be converted into energy and sustainable materials. Application of organic raw material chiefly aims at reducing the consumption of fossil-based items for daily human consumption. However, the most important challenge is associated with finding and developing proper biomass conversion and valorization methods. Although several technologies are being developed for the large-scale conversion of biomass into energy, their widespread adoption remains limited due to the requirement for high capital investment. Hydrothermal treatments, torrefaction, pyrolysis, gasification and combustion are preferred routes for the treatment and valorization of biomass and other organic residues [17]. Figure 2 shows the products from different thermochemical conversion techniques and identifies the major application fields of each product.

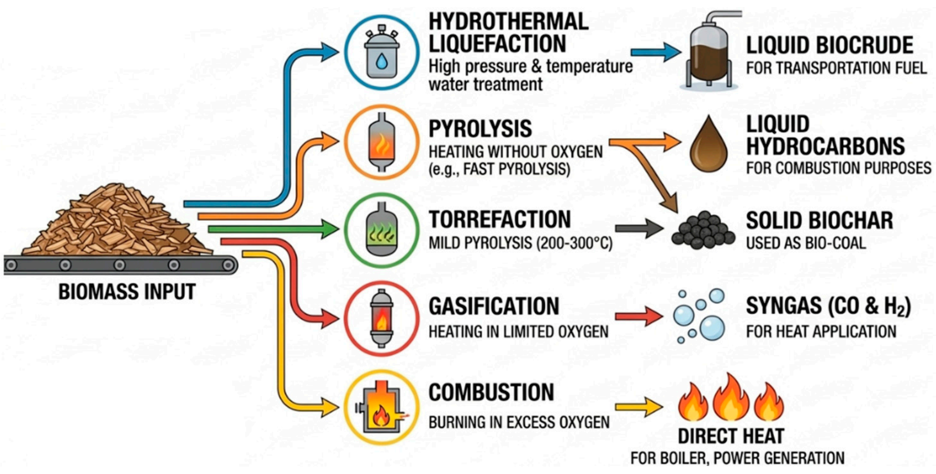

Figure 2. Thermochemical methods of biomass conversion into high-value hydrocarbons, for different applications**.**

Thermochemical conversion technologies enable the transformation of biomass into solid, liquid, and gaseous energy carriers through controlled variations in temperature, reaction conditions, and residence time. Among these pathways, pyrolysis is the most widely applied method, accounting for approximately 52 % of reported biomass-to-energy studies. Pyrolysis involves the thermal decomposition of biomass at elevated temperatures in the absence of oxygen, producing liquid bio-oil along with solid char and non-condensable gases, which are commonly utilized for energy generation and further upgrading. Hydrothermal processing, including hydrothermal liquefaction and hydrothermal carbonization, ranks as the second most reported conversion route with a share of about 11-12 %. Operating in hot, compressed water at temperatures typically between 200 and 500 °C, hydrothermal processing is particularly suited for wet biomass and organic residues. These processes yield high-energy-density liquid biocrude and solid hydrochar without the need for prior drying the feedstock. Combustion represents the third most practiced thermochemical pathway, accounting for roughly 10 % of applications, and remains a mature technology for direct heat and power generation [18,19]. Gasification and related high-temperature conversion routes are less frequently reported and involve partial oxidation of biomass under controlled oxygen conditions to produce syngas. Collectively, these thermochemical pathways show that adjusting reaction severity and operating conditions governs the distribution of solid, liquid, and gaseous products share during biomass conversion [20,21].

Thermochemical conversion technologies for biomass can be broadly categorized into conventional incineration (CI) and advanced thermal (AT) techniques. This classification is based on reaction conditions, operating severity, and desired product properties. CI techniques rely on the complete oxidation of biomass in excess oxygen to directly generate heat and electricity. In contrast, AT techniques operate under oxygen deficient or controlled environments [21–23]. These techniques are designed to enhance conversion efficiency while enabling the production of biofuels. These advanced approaches include pyrolysis, gasification, and related high-temperature processes distinguished by the extent of oxidation and the nature of products [24]. Pyrolysis proceeds in the absence of oxygen and favors the formation of liquid and solid products through thermal decomposition. Gasification, on the other hand, employs partial oxidation at higher temperatures to generate syngas (H_2 + CO) as the dominant product [25,26]. Hydrothermal routes extend this classification by introducing water as a reactive medium, enabling biomass conversion at elevated pressures and moderate temperatures. Within this advanced thermal framework, fast/flash pyrolysis and hydrothermal liquefaction (HTL) represent two distinct but complementary pathways that bridge conventional waste-to-energy and fuel-oriented biorefinery concepts. As highlighted in waste-to-energy classifications, pyrolysis emerges as a key advanced alternative to incineration due to its ability to recover liquid fuels rather than solely heat or power. Building on this foundation, comparative thermochemical analyses of fast/flash pyrolysis and HTL demonstrate that process selection is governed not only by operating conditions but also by the biochemical composition and moisture content of the feedstock [27].

3. Hydrothermal- Liquification, Biocrude Upgradation Techniques and Factors Affecting Biocrude Upgradation

Biomass is a chemically and physically heterogeneous material composed predominantly of organic matter, accompanied by a smaller but influential fraction of inorganic (mineral) constituents. The organic fraction is mainly responsible for energy content and reactivity. Biomass chiefly consists of carbon, hydrogen, and oxygen-rich compounds, with minor amounts of nitrogen, sulfur, and phosphorus, which influence emissions during conversion. The inorganic fraction in biomass comprises minerals present as organically bound elements, simple salts, or discrete mineral phases originating from plant uptake, soil contamination, or processing [28]. The compounds typically include alkali and alkaline earth metals (K, Ca, Mg, Na), silicon, phosphorus, chlorine, and trace elements. Compared to fossil fuels, bio-based liquid hydrocarbons are characterized by high oxygen content, high viscosity, and strong compositional variability. These properties collectively govern the heating value, conversion efficiency, and ash-related challenges in energy application of biofuels [28,29]. Hydrothermal processes, particularly HTL, represent a thermochemical conversion route that is fundamentally distinct from both conventional incineration and dry advanced thermal techniques. Incineration is designed for complete oxidation and direct heat or power generation, while dry advanced thermal routes, such as pyrolysis, aim to recover energy intermediates from low-moisture feedstocks [20,30]. HTL, in contrast, operates effectively on wet and compositionally heterogeneous biomass removing the cost of drying pre-treatment. Conversion proceeds through hydrolysis, decomposition, and repolymerization reactions in hot compressed water. These mechanisms favor the formation of liquid products with higher carbon retention and lower oxygen content than typical pyrolysis oils [20,31]. Figure 3 illustrates the different mechanisms occurring during the HTL of biomass, based on the different components of biomass. The figure indicates that proteins, lipids, carbohydrates, and lignin undergo a common initial hydrolysis step, forming reactive intermediates that follow component-specific secondary pathways under HTL conditions. Lipids and proteins preferentially contribute to bio-oil through fatty acid decarboxylation/dehydration and amino-acid deamination/decarboxylation, respectively. Carbohydrates hydrolyze to sugars that further fragment and dehydrate to yield water-soluble compounds in the aqueous phase, with partial decarboxylation producing gaseous products. Lignin degrades into phenolic intermediates that undergo repolymerization and condensation, leading predominantly to solid biochar formation [32–34]. While hydrolysis serves as the initial step in biomass conversion during the HTL process, the final product distribution is controlled by competing secondary reactions. Stabilization pathways promote bio-crude and gas formation, whereas condensation reactions preferentially direct carbon toward solid biochar, especially in lignin-rich feedstocks [35].

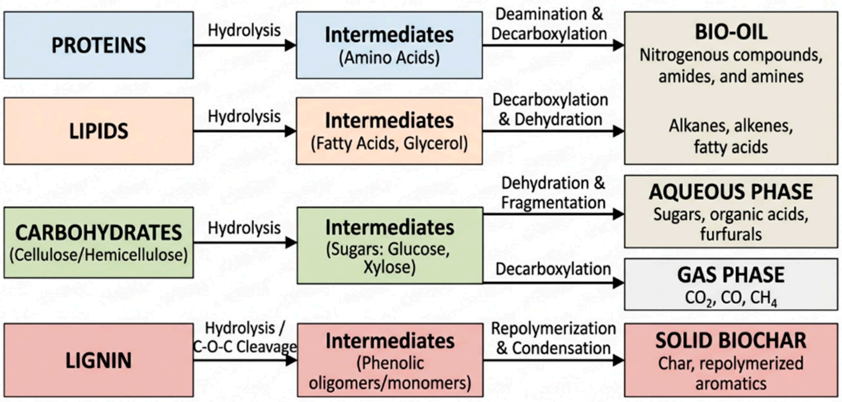

Figure 3. Schematic diagram of major HTL reaction pathways for specific components of lignocellulosic biomass feedstock.

The major energy producing biomass are obtained from wood processing residues, agricultural residues, food wastes, algal biomass, and municipal solid wastes [36]. However, biomass derived HTL biocrude has a limited application in commercial energy sector due to its physio-chemical limitations. These drawbacks require treatment through advanced techniques for improving the quality of the product. However, the intricacy of the process and complex chemical structure of biocrude, makes the upgradation task quite difficult for industrial application [37]. Figure 4 shows the compounds found in energy producing biomass. The quality and quantity of bio-crude produced by HTL are strongly rooted to the properties and composition of the biomass. Besides, lignocellulosic components (cellulose, hemicellulose and lignin) and extractives (proteins and lipids), presence of aldehydes, phenolic compounds, N-containing groups and esters, have significant impact on the quality of biocrude produced [38–40].

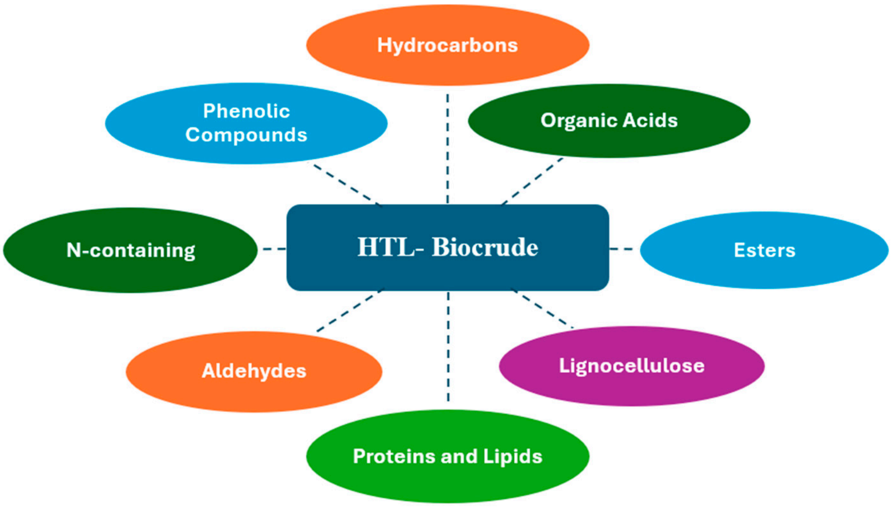

Figure 4. Major chemical compounds present in the HTL bio-crude.

The major upgradation techniques adopted for enhancing biocrude quality are divided into physical and chemical upgradation methods, depending on the nature of the method used for extracting usable fuels. Physical upgradation techniques like supercritical fluid treatment, solvent addition, emulsification and distillation, target the direct extraction of valuable hydrocarbons from biocrude. However, these techniques do not have any influence in enhancing the yield of usable hydrocarbons. Contrary to physical techniques, chemical treatments enhance the physical fuel properties of the biocrude and increase the hydrocarbon yield through molecular alterations, through selective removal of unwanted heteroatoms. The most adopted chemical techniques for biocrude upgradation are hydrotreating, esterification, catalytic cracking, and steam reforming [41]. Among these approaches, catalytic hydrotreating has emerged as the most extensively investigated route due to its effectiveness in heteroatom removal and its direct compatibility with existing petroleum refining infrastructure. Catalytic hydrotreating is a thermochemical upgrading process in which biocrude is treated in the presence of hydrogen to promote hydrogenation reactions. The process targets removal of heteroatoms through mechanisms like hydro-deoxygenation, hydro-desulfurization, and hydro-denitrogenation [42]. Table 1 compiles different studies conducted on upgradation of HTL-produced biocrude from different feedstocks through hydrotreatment techniques. The table summarizes catalytic upgrading studies of HTL biocrudes spanning lignocellulosic, lipid-rich, algal, and waste-derived feedstocks. It is observed that across all systems, sulfided NiMo and CoMo-based catalysts exhibit strong hydrodeoxygenation activity, yielding substantial reductions in oxygen content under a wide range of operating conditions.

Table 1. Comparison of catalytic upgradation of HTL biocrudes from feedstocks of different origin.

Feedstock	Dominant Issues	Upgrading Strategy	Catalyst Type	Operating Conditions (T, P)	Products	References
Forest residues (50/50 spruce-pine wood)	High O_2 (11 wt. %), phenolic compounds, higsh TAN (68 mgKOH g^{-1})	Solvent de-asphalting (n-pentane, toluene, DCM, EtOAc); Mild hydrotreating	Sulfided $NiMo/Al_2O_3$	290-320 °C, 9 h, 1400 psi H_2	Distillate-range hydrocarbons; O_2 final 2.9 wt. %	[43]
Co-HTL of wheat straw + waste cooking oil	High oxygen (10 wt. %), high acidity.	Batch hydrodeoxygenation	Sulfided $NiMo/\gamma Al_2O_3$	350 °C, 8 h, 1500 psi H_2	Diesel-range paraffins (C17–C19); O_2 final 0.56 wt. %.	[44]
Wastewater-grown microalgae	High heteroatoms (O, N, S), aromatic-rich oil.	One-step HTL + in-situ catalytic upgrading	$NiMo/Al_2O_3$	320-370 °C, 30-120 min, 18-22 MPa	Aromatics + alkanes; SAF precursor; O_2 final 5-10 wt% O_2.	[45]
Sewage-sludge HTL biocrude	Extremely high N (6-7 wt.%), refractory carbazoles/indoles	Severe batch hydrotreatment	$NiMoS/Al_2O_3$	350-390 °C, 0-5 h, 100 bar H_2	Fuel-range liquids (73 wt% <350 °C); N_2 residual of 1.4 wt%, high degree of O_2 removal	[46]

Food waste and sewage-sludge	High N (4-5 wt.%), high metals, catalyst stability concerns	Continuous two-stage hydrotreating (guard+ main bed)	$CoMo/Al_2O_3$ (guard) + $NiMo/Al_2O_3$ (main)	350-400 °C, 1500 psi, WHSV 2 h^{-1}	Diesel-rich blend stock (70% diesel cut); 0.15-0.25 wt.% O	[47]

The table suggests that feedstocks dominated by lignin or lipid-derived oxygenates reach low residual oxygen levels at moderate severity. In contrast, biocrudes derived from sewage sludge, food waste, and wastewater-grown biomass show persistent nitrogen-related challenges despite severe reaction conditions. Multi-stage configurations and guard-bed deployment reported for nitrogen and metal-rich feeds reflect catalyst protection and stability attainment with very low O_2 concentration. The data collectively indicate that oxygen removal is kinetically favorable over conventional hydrotreating catalysts. However, nitrogen-containing species have higher severity demands, require well designed upgrading strategies and longer catalyst lifetime. The following sections elaborate on the different hydro-processing technologies used at industrial levels for enhancing the quality of crude oil, and thus, increasing the amount of liquid fuel yield.

3.1. Hydro-Processing Methods of HTL-Biocrude

Hydrotreatment of crude oils has been practiced at commercial refineries for several decades to produce high-quality transportation fuels. It is primarily divided into three major categories: (i) hydrodeoxygenation (HDO), (ii) hydrodenitrogenation (HDN), and (iii) hydrodesulfurization (HDS). As suggested by their nomenclature, these processes selectively remove heteroatoms such as oxygen, nitrogen, and sulfur, present in both conventional petroleum crudes and renewable biocrudes, respectively. The feedstock is processed under elevated temperature and hydrogen pressure, converting heteroatoms into by-products such as water (H_2O), hydrogen sulfide (H_2S), and ammonia (NH_3), while simultaneously improving fuel quality and stability [48,49]. A common way to see and understand the hydrotreatment reaction is shown in equation (1) [50].

$$feed + H_2 \rightarrow hydrocarbon + H_2S + NH_3 + H_2O \quad (1)$$

However, the high severity of operating conditions, required for processes like HDN and HDS, limits their application at commercial levels for biocrude upgradation. Nevertheless, HDO processes require less severe conditions, to remove elemental oxygenated compounds from bio-based crude oils. The differences in the nature of the upgradation processes favor the use of oxygen containing biomass for fuel production as compared to nitrogenous compounds. Thus, further discussions in this article would focus on the research developments in HDO processes to understand its applicability and limitations faced in the industries.

3.2. Hydrodeoxygenation

Hydrodeoxygenation is a key upgrading reaction for biomass-derived crude oils, enabling the removal of oxygenated compounds through hydrogenation and hydrogenolysis reactions. In HDO, C-O-C, C-O-H, and C-O bonds, present in phenols, aldehydes, ketones, acids, and ether groups, are cleaved with oxygen predominantly eliminated as water. However, the process ensures that the hydrocarbon framework is retained or hydrogenated depending on reaction conditions and catalyst properties [51]. Conventional HDO processes are conducted at moderate to high temperatures (typically 300-400 °C) and elevated hydrogen pressures over heterogeneous catalysts. The efficiency of HDO is governed by the balance between metal sites, responsible for hydrogen activation, and acid sites to carry out dehydration, C-O bond scission, and ring-opening reactions [52,53].

The reaction environment plays a critical role in determining HDO performance, particularly when comparing monophasic and biphasic solvent systems. In monophasic systems, solvent, and catalyst exist in a single liquid phase, where reaction rates and selectivity are strongly influenced by solvent polarity and solubility effects. Single-phase systems offer simplified reactor design and easier catalyst handling, but are prone to secondary reactions like repolymerization, coke formation, and catalyst deactivation, especially at the high temperatures [53]. In contrast, biphasic water-oil systems introduce a simultaneous reaction-separation function. These systems increase the interfacial area between phases, promote selective partitioning of reactants and products, and suppress undesired side reactions by continuously extracting products into the organic phase. Studies approve that biphasic systems improve mass transfer, stabilize transition states, and reduces catalyst deactivation, and hydrolysis rates of sensitive intermediates [53–55].

Recent advances emphasize the use of tailored catalysts in conjunction with biphasic systems to further enhance HDO efficiency. Amphiphilic and carbon-based catalysts can stabilize water-oil interfaces, forming Pickering emulsions to maximize interfacial contact and hydrogen availability at the reaction zones. Noble metal catalysts exhibit high hydrogenation activity under relatively mild conditions, while non-noble metal systems and bifunctional catalysts enable cost-effective large-scale deployment [48,52,56,57]. Further, studies related to model compounds demonstrate that biphasic HDO systems enhance selectivity toward deoxygenated products, improve catalyst stability, and simplify downstream separation by coupling reaction and extraction within a single process step [53,58–60]. Collectively, these developments position HDO as a robust and scalable strategy for upgrading oxygen-rich biocrudes into fuel-compatible intermediates in biphasic reaction environments.

Several studies have been conducted to help explore the impact of catalytic and non-catalytic HDO processes for upgradation of biocrude oils. Table 2 lists different studies conducted on HDO of bio-based crude oils produced through HTL process. The table indicated that deep deoxygenation of HTL biocrudes requires high-temperature (330-400 °C), and abundant hydrogen supply (70-150 bar) for upgradation. Across diverse feedstocks, achieving oxygen contents below 1 wt.% typically requires sulfided NiMo, CoMo, or noble metal catalysts. Further, batch hydro treatment studies rely on high catalyst loadings (10-40 wt.%) to compensate for limited residence time and mass-transfer constraints [61,62].

Table 2. Studies on hydrodeoxygenation of HTL produced biocrude from different sources.

Feedstock	**Upgrading strategy**	**Catalyst used (loading in wt.%)**	**Operating conditions**	**Observation**	**Ref.**
High boiling fraction of Soyabean straw HTL biocrude	Catalytic hydrotreatment in H_2-donor solvent (tetralin + decalin)	Pt/C (40 wt.%)	T = 400 ºC, Pr. = 100 bar t = 4h	98.6% S, 96.2% N, 87.1% O_2 removed	[61]
HTL biocrude of Animal carcass (streaky pork)	Catalytic hydrotreatment of biocrude in a water-free system	CoMo/γAl_2O_3 (20 wt.%)	T = 400 ºC, Pr. = 150 bar t = 4h	64.4% N, 84.6% O_2 removed	[62]

HTL biocrude of Food waste (mixed vegetables + ground meat)	Single-step catalytic HDO, HDN, and mild hydrocracking	Pd/C (20 wt.%)	T = 350 ºC, Pr. = 30 bar t = 3h	58% O_2 removed, low H_2 consumption	[63]
HTL biocrude derived from Microalgae (*Nannochlopsis*)	Catalytic hydrodeoxygenation (HDO) following non-catalytic HTL	NiMoC/AC (10 wt.%)	T = 400 ºC, Pr. = 30 bar t = 2.75h	94% O_2 reduction, 72.5% oil yield, 43 MJ/kg HHV	[64]
HTL biocrude of municipal sweage sludge	Single-step HDO of solvent-extracted biocrudes (DCM, hexane, toluene, acetone)	Ni/SiO_2-Al_2O_3 (5 wt.%)	T = 350 ºC, Pr. = 70 bar t = 1h	Hexane extract: 5 wt. % O_2; Toluene extract 12 wt. % O_2	[65]
HTL biocrude of bio-pulp derived from food wastes.	2-stage continuous catalytic HDO using trickle-bed reactors with guard-bed stabilization followed by deep hydrotreating	Mo/Al_2O_3 (guard bed- 60 g) + NiMo/Al_2O_3 (main catalyst 47 g)	Continuous process; 1st stage: 260 °C, 2nd stage: 400 °C; 10 MPa H_2, WHSV 0.2 h^{-1}	Upgraded oil yield of 92 wt.%, 64% diesel production, 96% O_2 removed.	[66]
Partially hydrotreated HTL biocrude from a 50/50 spruce-pine wood mixture	Partial HDO to render biocrude fully miscible in VGO, followed by 2-stage co-processing	Hydrotreating: 15 mL NiMo catalyst with 28 mL SiC; Hydrocracking: 10 mL Zeolite-based catalyst with 18.5 mL SiC	Hydrotreating: T = 330 ºC, Pr. = 100 bar WHSV = 0.5 h^{-1}; Hydrocracking: T = 405 ºC, Pr. = 100 bar LHSV = 1.5 h^{-1}	Partially HDO biocrude: 3.6 wt. % O_2. co-processed blend: 0.16 wt. % O_2	[67]
HTL biocrude derived from spent coffee grounds	Mild hydrotreatment (HDO stabilization) followed by refinery-relevant coprocessing	Sulfided NiMo/γAl_2O_3 (7.1 v/v blend with demetallization catalyst)	T = 330 ºC, Pr. = 70 bar LHSV = 1 h^{-1}	0.39 wt. % O_2 in stabilized biocrude	[68]

Model compounds of HTL biocrude, derived from black liquor	Catalytic HDO in subcritical/supercritical water	Activated Carbon supported NiMoSx (6.5 wt.%)	T = 380 ºC, Pr. = 15 bar t = 2 h	Highest selectivity to phenols. 40% degree of deoxygenation for both conditions	[69]
HTL biocrude mixture of wheat straw and waste cooking oil	Single-step HDO	Sulfided NiMo/γAl_2O_3 (13 wt.%)	T = 350 ºC, Pr. = 103 bar t = 8 h	Final O_2 content 0.6 wt.%, HHV of 46 MJ/kg, and low acidity	[70]

Contrary to the batch processes, studies on continuous trickle-bed hydrotreatment and staged upgrading strategies showed similar or superior oxygen removal at lower catalyst loading [66,67]. H2-donor solvents and partial HDO steps further mitigate coke formation and improve stability at high severity. Nevertheless, upgrading performance strongly depends on feedstock composition and strategy selection [62,65]. Protein and nitrogen-rich biocrudes required more severe hydrotreatment yet still exhibited limited nitrogen removal. This indicates that HDN remains more challenging to accomplish than HDO at lab-scale studies [62]. Lignocellulosic and lipid-rich feeds respond more favorably to both single-step HDO and staged upgrading approaches. However, partial HDO prior to co-processing of lignin rich feedstock derived biocrude reported higher miscibility and characteristics of stable refinery integration. Besides, subsequent refinery hydro-processing further reduces biocrude oxygen content to fossil-like levels (< 0.2 wt.%) [67].

Hydrothermal liquefaction (HTL) biocrude is currently being recognized as a chemically multifunctional intermediate suitable to produce biochemicals along with fuels. Chemically, HTL biocrude comprises a highly heterogeneous mixture of phenolic monomers and oligomers, carboxylic acids, ketones, aldehydes, esters, fatty acids, olefinic hydrocarbons, and N and S-containing heterocycles. The chemical compounds are majorly formed through hydrolysis, dehydration, decarboxylation, retro-aldol condensation, and recombination reactions under subcritical and near-critical water conditions [71,72]. In lignocellulosic feedstocks, lignin depolymerization via β-O-4 ether bond cleavage yields guaiacols, syringols, catechols, and alkyl phenols. This process generates phenolic-rich biocrudes that have demonstrated direct applicability as renewable substitutes for petroleum phenol in phenol-formaldehyde resins and wood adhesives [73–75]. Concurrently, cellulose and hemicellulose hydrolysis followed by dehydration reactions produce furfural, 5-hydroxymethylfurfural (5-HMF), levulinic acid, and short-chain organic acids. These chemicals function as platform molecules for downstream synthesis of resins, plasticizers, solvents, pharmaceutical intermediates, and agrochemicals [72,73]. Lipid-rich feedstocks undergo triglyceride hydrolysis, subsequent decarboxylation and hydrogen transfer reactions, yielding free fatty acids, fatty esters, and long-chain hydrocarbons. This enables targeted recovery of specialty chemicals, lubricants, surfactants, and oleochemical applications without the need of attaining deep hydrotreating severity [73,76,77]. Protein-derived biocrudes introduce amine, amide, pyrrolic, pyridinic, and nitrogen species formed through deamination and Maillard-type reactions. These chemical compounds are valuable precursors for pharmaceuticals, corrosion inhibitors, functional additives, and specialty reagents post separation [72,73,78]. The heavy biocrude fraction (boiling range >350 °C) contributes as a potential source of bio-asphaltenes and bio-polyol precursors, supporting applications in bitumen modification, polymer synthesis, and polyurethane production

[79,80]. Importantly, HTL biocrude valorization is enhanced by integration with the aqueous phase, which contains water-soluble carboxylic acids, alcohols, sugars, and nitrogenous compounds. These compounds can be recovered for chemical use or nutrient recycling (fertilizers), improving overall carbon efficiency and process circularity [81–83].

Besides producing liquid products, the HTL process also produces a significant quantity of solid by-products known as hydrochar. It is carbon-rich source that has been identified as a promising resource for several applications like soil enrichment, water treatment and many more. The following section carries out a detailed discussion of the chemical composition of the solid hydrochar along with a comprehensive discussion on the promising routes of its applications.

4. Applications for Hydrochar Produced from Hydrothermal Liquification

Hydrochar is a carbon-rich solid material produced through hydrothermal conversion of biomass in subcritical or supercritical water. Thus, making hydrochar production particularly suitable for wet biomass without an energy-intensive drying step. Unlike biochar, hydrochar is generated at relatively low temperatures (typically 180-240 °C) under autogenous pressure [84,85]. Hydrothermal carbonization (HTC) is the most widely adopted method for the production hydrochar globally. HTC produces hydrochar through the compression of water in the medium at temperatures lower than the pyrolysis range. However, at temperature higher than 260 °C HTL is the major process employed for hydrochar making [84,86,87]. HTL process promotes dehydration, decarboxylation, and polymerization reactions, yielding the solid by-product, hydrochar. As a result, hydrochar typically exhibits higher H/C and O/C ratios, lower ash content, and a more acidic surface compared to pyrolysis-derived biochar [88,89]. Figure 5 illustrates different methods of hydrochar production, as found in literature. The image lists the important conditions needed during each process, for hydrochar production. Lower temperatures and pressure are both favorable to achieve high yields of hydrochar in HTC. However, with the increase in temperature and pressure, the major product of hydrotreating process shifts towards liquid or gas-based resources, with limited amount of hydrochar production [87].

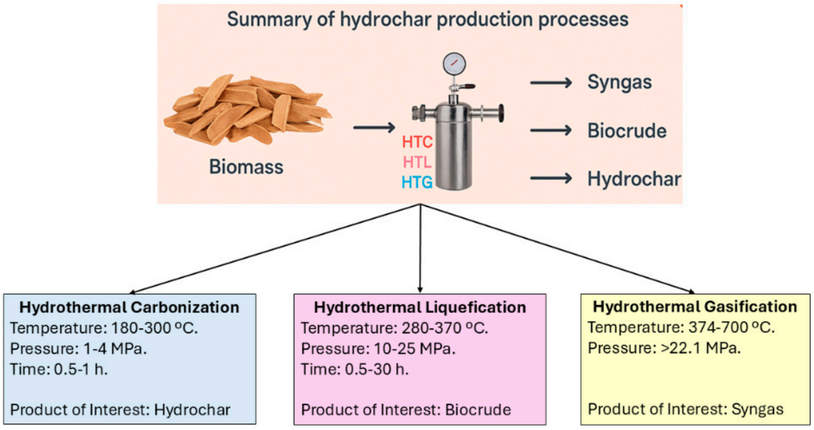

Figure 5. Methods and parameters of hydrochar production (Adopted and modified from [87]).

Although pristine hydrochar generally possesses low surface area and porosity as compared char produced through other techniques. However, the physicochemical properties of hydrochar can be significantly tuned through processes like activation and functionalization [90,91]. These characteristics have positioned hydrochar as a promising renewable material for applications in catalyst production, adsorption applications, carbon sequestration, and environmental remediation [88]. The following section contains a brief discussion on the different applications of hydrochar upon specific physio-chemical treatments.

4.1. Bio-Coal for Energy

Hydrochar contains a high fraction of fixed carbon and a reduced oxygen content compared with raw biomass, leading to improved fuel quality and greater energy density. The elemental composition of hydrochar typically shows lower O/C atomic ratios than untreated biomass, indicating a higher degree of carbonization and enhanced calorific value [92]. As a result, hydrochar commonly exhibits higher heating values in the range of low-rank coals, with values often comparable to lignite and, while in some cases, approaching those of bituminous coal [93,94]. The increased carbon content and reduced volatile matter of hydrochar contribute to more stable and efficient combustion behavior. The product also contains fewer inorganic constituents than many raw biomasses, which results in lower ash content and improved combustion cleanliness. These chemical characteristics support smoother ignition, reduced slagging tendencies, and improved overall fuel performance [95,96]. Consequently, hydrochar can be used as a solid fuel for stationary energy generation, either as a standalone fuel or in co-firing systems with coal, without major modifications to existing infrastructure.

In addition to direct combustion, the chemical composition of hydrochar makes it a well-suited feedstock for gasification. The high fixed-carbon content and reduced volatile matter, shifts gasification of hydrochars from volatile-dominated reactions to char controlled heterogeneous reactions. Elemental analysis shows increased carbon content and decreased hydrogen and oxygen contents, resembling a coal-like structure. This carbon-dense composition promotes the formation of condensed aromatic structures that are thermally stable and reactive during char-steam and char-CO_2 gasification [97]. The enrichment of fixed carbon enhances hydrogen production through char gasification and the water-gas shift reaction. At the same time, the removal of O2-containing functional groups suppresses excessive CO_2 formation and reduces hydrogen consumption, leading to improved syngas quality and low tar production [98,99]. In addition, alkali and alkaline earth metals such as K, Ca, and Mg are relatively enriched in the solid phase and act as intrinsic catalysts for gasification and tar reforming [96]. Together, the high fixed-carbon content, increased aromaticity, reduced oxygen functionality, and favorable inorganic composition explain the coal-like energy containment for efficient syngas production in hydrothermally derived char.

Several studies have been conducted to find the potential of bio-coal production from hydrothermal processes over a long period of time. These studies majorly focused on application of HTC as a biomass conversion process. A research study carried out by Musa et al. in 2022 analyzed the effect of process variables on biocoal production through HTC of pine Kraft lignin at low temperatures. The study observed that, lignin-rich feedstocks exhibit a high degree of coalification under HTC. During HTC of pine Kraft lignin, the solid product retained a large fraction of aromatic carbon because lignin contains pre-condensed phenylpropane units. Further, hydrolysis cleaved ether and ester linkages, while dehydration and decarboxylation preferentially removed oxygen rather than carbon. Solid-state 13C-NMR confirmed loss of oxygenated functional groups and enrichment of aromatic carbon in the solid phase. As a result, carbon recovery remained high even at elevated temperatures, and fuel ratios increased substantially with residence time. Alkali metal leaching occurred concurrently due to subcritical water acting as an effective inorganic solvent, improving ash behavior without compromising carbon retention [100]. A study focused on understanding the feasibility of bio-coal production through HTC in Malaysia, found that considering the Malaysian food waste composition, HTC is a suitable process for bio-coal production. However, it was observed that due to large moisture content of the feed, the fuel produced was found to be of moderate quality with limited improvements in combustion properties. Thus, concluding that, economic feasibility, rather than chemical limitation, emerged as the primary constraint for industrial adoption of HTC to create bio-coal [101]. A recent study conducted by Alper et al. (2024) investigated the production of bio-coal in presence of two sulfonic-acid catalysts, from lignocellulosic biomass, through HTC. The study observed that acid addition increased proton availability, promoting breakdown of polysaccharides into furanic intermediates, that polymerized into fixed carbon. Higher fuel ratios resulted, alongside increased formation of organic acids in the aqueous

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phase. Morphological cracking observed by electron microscopy corresponded to intensified volatile matter release, rather than thermal sintering [102]. Besides these studies, a study on HTC of Miscanthus, showed that HTC corrected biomass specific limitations unrelated to carbon content. Early harvested material suffered from high alkali concentrations and poor grindability. Thus, due to uneven particle sizes, HTC selectively removed inorganic species and disrupted fibrous structures, producing friable solids with coal-like combustion behaviour [103]. However, in another study on bio-coal production from elephant dung, torrefaction of feedstock produced limited coalification. Oxygen remained structurally bound, and energy demand was dominated by moisture evaporation. These results highlighted water-mediated chemistry as the critical factor enabling deep transformation in wet biomass systems [104].

Conclusively, hydrothermal processes produce a carbon-rich, coal-like solid (hydrochar) with enhanced fuel properties. The high fixed carbon, low O/C ratio, and heating values are comparable to low-rank coals, supporting efficient combustion and syngas generation. However, the degree of coalification achieved is strongly feed-dependent and is ultimately limited by techno-economic factors rather than chemistry alone.

4.2. Soil Enrichment

Hydrochar amendment modifies soil behavior primarily through surface chemistry and carbon fraction composition rather than through surface area or porosity. Multiple studies show that hydrochars rich in oxygen, nitrogen, and phosphorus containing functional groups interact directly with soil minerals, contaminants, and microorganisms [105,106]. These surface groups determine electrostatic interactions, chemical complexation, redox reactions, and mineral bridging. Thus, indicating that soil responses depend more on chemical reactivity than on bulk physical properties such as BET surface area [107,108]. Metal immobilization by hydrochar follows metal-specific pathways rather than a single universal mechanism. In lead-contaminated soils, phosphorus-enriched hydrochars immobilize Pb predominantly through the formation of insoluble Pb-phosphate phases and inner-sphere complexation with phosphate and carboxyl containing surface groups. This process sharply reduces Pb leaching and plant uptake, even under extreme contamination levels [106,109]. Other metals like chromium show significantly different fundamental behavior, compared to Pb contaminants. In a study on algal-derived hydrochar application for Cr removal, it was observed that the hydrochar promotes electron transfer from nitrogen-doped aromatic structures. This phenomenon reduces Cr (VI) to Cr (III), by subsequent immobilization through surface complexation and precipitation. Cadmium, however, shows weaker immobilization because it lacks redox chemistry and relies mainly on electrostatic attraction and coordination with oxygen and nitrogen-containing functional groups. These results highlight that hydrochar effectiveness depends on matching hydrochar chemistry with metal speciation [110].

Hydrochar also improves soil physical structure by enhancing soil aggregation. Experimental studies demonstrate that hydrochar accelerates macroaggregate formation by acting as nuclei for particulate organic matter while stimulating microbial production of binding agents [107,111]. Labile dissolved organic carbon initiates microbial activity, whereas aromatic carbon fractions become physically protected within aggregates. As a result, mean weight diameter increases by up to 100%, and soil organic carbon (SOC) increases by more than 140%, exceeding responses observed with straw or biochar amendments [107]. Nutrient retention and availability are similarly governed by surface chemistry. Hydrochars with high densities of acidic functional groups exhibit increased cation exchange capacity, improving ammonium and potassium retention and reducing nutrient leaching [112]. Nutrient release shifts from rapid dissolution to diffusion and sorption-controlled behavior. In fertilizer systems, hydrochar prolongs nitrogen residence time in soil while sustaining plant uptake and minimizing nutrient loss [108]. In alkaline soils, hydrochar enhances phosphorus availability by lowering pH and promoting microbial transformation of stable calcium-phosphate pools into labile forms [113]. Hydrochar amendments enhance soil aggregation, soil organic carbon protection, and nutrient retention when carbon remains accessible to microbial processing. Several studies indicate that carbon stability alone does not guarantee improved biological function, also, nutrient availability and microbial responses depend strongly on hydrochar chemistry and soil context. Thus, improving soil aggregation, SOC protection, and nutrient turnover [114–116].

Hydrochar performance varies with its physicochemical characteristics and the properties of the receiving soil. Under appropriate conditions, hydrochar immobilizes metals through chemical precipitation, redox transformation, and surface complexation. Subsequently, it also contributes to soil aggregation, soil organic carbon stabilization, and nutrient retention via interactions with soil minerals and microbes. However, the relative contribution of these processes differs across hydrochar types and soil systems. Thus, reflecting differences in surface functionality, carbon composition, and nutrient chemistry. This variability indicates that hydrochar behavior is context dependent and should be evaluated with consideration of both material properties and site-specific soil constraints.

4.3. Catalysts from Hydrochar

In recent years, biomass-derived carbon materials have been widely investigated as heterogeneous catalysts for energy and environmental applications. Among these, hydrochar has attracted growing attention due to the ease with which its surface chemistry can be deliberately modified to introduce catalytic functionality [88,117]. Several studies demonstrate that hydrochar can be transformed into effective solid catalysts or catalysts support, used for biofuel production, advanced oxidation processes, and biocatalysis, through post-synthetic chemical treatments [118–120]. Catalytic performance found across studies is closely linked to the physical and chemical characteristics of functionalized hydrochar. Surface roughness and accessible pore structures facilitate effective mass transfer and exposure of reactants to active sites [121,122]. Although hydrochar exhibits moderate surface areas compared to activated carbon, catalytic activity is primarily governed by the surface functional groups, along with the adsorption capacity [121]. Surface oxygen-containing functionalities on hydrochar enable post-synthetic functionalization, supporting the formation of basic catalytic sites through alkaline activation [121], stable Brønsted acid sites via sulfonation [123], and in covalent anchoring of enzymes following crosslinking [122].

Beyond acid-base catalysis, hydrochar has been applied in redox-driven water treatment systems. Yu et al. [124] in their study related to development of Fe-hydrochar composites to catalyze estrogen through Fenton-like mechanisms, demonstrated that Iron-loaded hydrochar effectively promoted Fenton-like oxidation. The modified hydrochar facilitated electron transfer and stabilized iron species during hydrogen peroxide activation [124]. Further, Li et al. (2022), extended this approach by developing hydrochar-based photocatalytic composites, achieving efficient pharmaceutical degradation under visible light [125]. These studies confirm that hydrochar contributes directly to catalytic mechanisms by mediating redox reactions rather than functioning solely as an adsorbent. Hydrochar has also been explored as a catalyst support for metal-based and biocatalytic systems. Pereira et al. (2022) synthesized a triazole-functionalized hydrochar to anchor palladium nanoparticles for ullmann coupling. They observed that triazole groups introduced onto hydrochar via CuAAC click chemistry, enabled uniform anchoring of palladium nanoparticles. This phenomenon resulted in a monodispersed, recyclable nanocatalyst that delivered high conversion and selectivity in Ullmann homocoupling reactions. The catalyst had high performance under mild, environmentally benign conditions, with minimal loss of activity over multiple reuse cycles [126].

The use of hydrochar as catalysts for biodiesel production has also been a burning topic of discussion in the bio-fuel engineering field. In a study conducted by Khan et al. in 2024 rice husk derived hydrochar was modified via cobalt impregnation to create a metal-anchored catalyst with high accessibility of active sites. The resulting RHAC-Co catalyst achieved biodiesel conversion efficiencies above 96% under relatively mild conditions (75 °C, low catalyst loading). This observation confirmed that the oxygen-rich hydrochar surface effectively stabilizes metal species and promotes transesterification activities [127]. Furthermore, in a dual-function system, mustard husk hydrochar coated with polyaspartic acid and incorporated with Fe-Mn species was designed to address both heavy-metal remediation and hydrogen evolution. The modified hydrochar showed exceptional Pb

(II) removal (approx. 99%) and significantly enhanced H2 generation rates. This observation was attributed to increased surface area, improved electron transfer, and negatively charged oxygen-containing functional groups that favored metal binding and redox reactions [128].

Hydrochar has also shown strong catalytic performance in oxidation-based water treatment processes. Glucose-derived hydrochar combined with bimetallic metal-organic frameworks (MOFs) enabled efficient activation of peroxymonosulfate. Thus, resulting in rapid dye degradation and high mineralization efficiency over a wide pH range. It was observed that the hydrochar improved the structural stability of the MOF and suppressed metal leaching, extending catalyst lifetime [129]. Similarly, Fe-activated hydrochar produced from olive mill waste was evaluated in photo-Fenton systems, where it promoted hydroxyl radical generation and achieved rapid decolorization of both synthetic dyes and real textile wastewater while maintaining activity over repeated cycles [130]. In another photocatalytic study, hydrochar derived from ice-cream wastewater was used as a conductive support for TiO_2 nanoparticles. The composite exhibited nearly complete dye degradation due to inhibited nanoparticle agglomeration and reduced charge-carrier recombination, with hydrochar acting as an electron reservoir [131].

Although hydrochar's catalytic performance is widely attributed to surface functional groups, porosity, and metal-support interactions, its intrinsic electronic behavior remains inadequately addressed. In several redox-driven applications, including photocatalysis, Fenton like oxidation, and hydrogen evolution, hydrochar is frequently reported to promote electron transfer or function as an electron reservoir. However, these roles are largely inferred from enhanced catalytic activity rather than supported by direct evaluation of charge-transport properties. Electronic conductivity and internal charge transfer within the hydrochar matrix therefore emerge as critical yet insufficiently characterized factors governing catalytic performance.

Biomass has been used for synthesis of several value-added products, especially in the material science and energy industry. Thus, there are numerous techniques that are adopted in the industry or lab scale studies, to broaden the scope of biomass valorization. A few methods like pyrolysis, gasification, hydrothermal liquefication, Fischer-Tropsch reaction, anaerobic digestion etc., have been studied widely in the biomass valorization industry, and adopted at commercial levels. Figure 6 illustrates a technology readiness level (TRL) scale of important biomass to energy conversion techniques, widely studied in recent years [132]. The image enlists TRL rankings of these techniques in 2024, for energy production applications only.

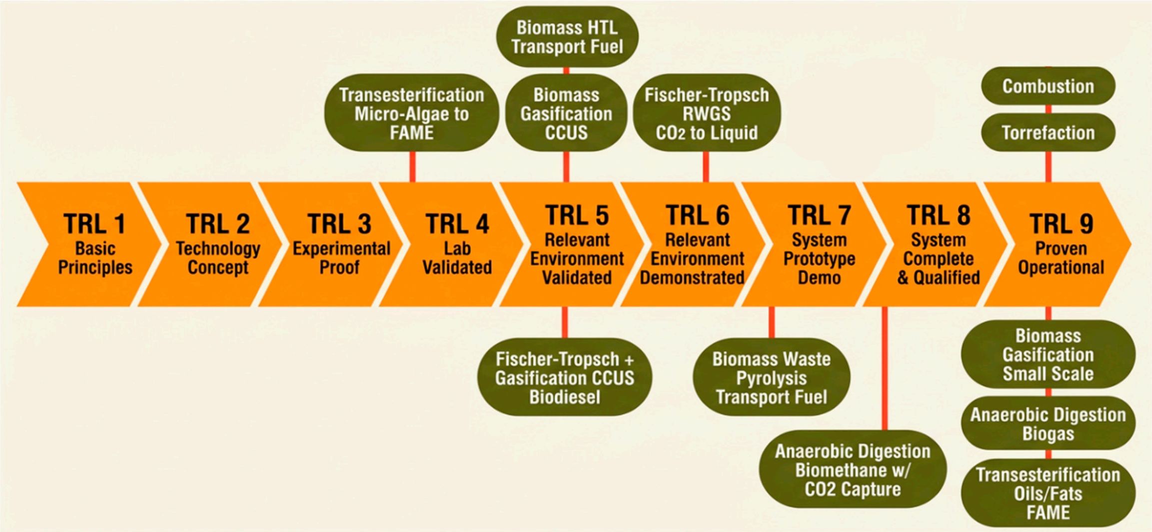

Figure 6. TRL scores of thermochemical routes for biomass valorization in 2024.

The image shows that processes at early-to-mid development include micro-algae transesterification to fatty acid methyl esters (TRL-4). Techniques like biomass hydrothermal

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liquefaction for transportation fuels, biomass gasification integrated with carbon capture and storage (CCUS), and Fischer–Tropsch synthesis coupled with gasification and CCUS are listed in TRL 5 scores, signifying their validation at relevant systems. Further, CO_2-to-liquid fuels production via Fischer–Tropsch synthesis and reverse water-gas shift (RWGS) is shown at TRL-6, reflecting demonstration under relevant conditions.

Notably, advanced technologies include biomass waste pyrolysis for transportation fuels (TRL 7) and anaerobic digestion to biomethane with CO_2 capture (TRL 8). Fully mature, commercially deployed routes (TRL 9) comprise anaerobic digestion to biogas, small-scale biomass gasification to produce bio-syngas, torrefaction, combustion, and transesterification of oils and fats to FAME, highlighting their established operational readiness relative to emerging pathways. The TRL analysis reveals that conventional biomass conversion pathways are commercially mature. Yet advanced fuel synthesis and CCUS-integrated processes remain at intermediate readiness due to scale-up and integration challenges. Consequently, near-term deployment will be driven by established technologies (AD for biomethane, biomass pyrolysis, etc.), whereas mid-TRL pathways (CCUS integrated techniques) require focused development to improve system integration, cost competitiveness, and long-term operability.

The development in adopting these techniques can be enhanced through the integration of artificial intelligence and machine learning techniques for characterization of feeds, operating conditions and products. The following section carries out a detailed literature review of different studies implementing AI/ML techniques in biomass valorization.

5. Application of Artificial Intelligence and Machine Learning in Biomass Valorization

The valorization of biomass into fuels, chemicals, and energy carriers involves inherently complex and nonlinear processes operating across multiple spatial and temporal scales. These systems are strongly influenced by feedstock heterogeneity, reaction pathways, and tight coupling between operating parameters. Conventional mechanistic and empirical models often struggle to represent such complexity with sufficient accuracy, particularly under realistic conditions. Additionally, experimental datasets are limited, and feedstock properties vary significantly between sources. As a result, the predictive capability and applicability of conventional models to process optimization and scale-up strategies remain constrained [133,134]. In recent years, artificial intelligence (AI) and machine learning (ML) techniques have emerged as effective tools to address these limitations. Unlike traditional modeling approaches, AI/ML methods can directly learn nonlinear relationships from experimental and operational data without requiring explicit assumptions about reaction mechanisms [135]. This capability makes them well suited for handling multivariable interactions, complex nonlinear behavior, and high-dimensional datasets commonly encountered in biomass conversion systems [136]. Consequently, AI-based models have been increasingly employed for prediction, optimization, and decision support in biomass valorization pathways. Broadly, AI/ML applications in biomass valorization span four interconnected domains: (i) prediction of biomass availability and properties, (ii) modeling and optimization of biochemical and thermochemical conversion processes, (iii) yield, and quality prediction for biofuels, and (iv) system-level integration encompassing supply chains, life cycle assessment (LCA), and techno-economic analysis (TEA) [133,137]. Several studies have been carried out in recent years to analyze the scope of implementing AI/ML applications in biomass valorization methods, especially for predicting the yield of targeted products, or product qualities. A few of these studies are listed below in Table 3 that provides an overview of AI/ML applications across major biomass valorization pathways, revealing consistent performance trends and shared limitations.

Table 3. Comparative study for different AI/ML implemented studies in biomass valorization.

Category of Study	Primary Objective	AI/ML model	Key Observations	Limitations Observed	Reference
Syngas Production	Optimize hydrogen-rich syngas from aqueous phase reforming (APR).	Artificial Neural Networks (ANN)	Catalyst type and temperature are the dominant variables for H_2 selectivity. 90% of predictions lay within ±5% error of experimental values.	ANN performance fluctuates with extreme pressure variations.	[134]
Algal Biofuels production	Optimize HTL and HTG for bio-oil and hydrogen production.	Combined machine learning based Tunable Decision Support System and Tunable Recommendation System	AI-optimized parameters deviated by < 3% from experimental optima. Required experimental runs reduced by 65% compared to manual trial-and-error optimization	Nonlinearity in supercritical water gasification. Prediction confidence intervals and robustness under noisy data were not formally assessed	[138]
Feedstock Characterization	Predict HHV of biomass fuels through ML models	Linear regression, Random Forest, Extreme gradient boosting (XGBoost), adaptive	ML outperforms linear regression, XGBoost gives best performance across training datasets.	The model functions as a screening tool rather than offering dynamic optimization. Variability due to	[139]

		boosting (AdaBoost		experimental protocols is not normalized.	
Pyrolysis Kinetics	Develop ML-models to predict biomass pyrolysis kinetic parameters	ANN models and a hybrid Particle Swarm Optimization (PSO-ANN) approach	PSO significantly improved ANN training stability. Maximum relative deviation decreased from 12.85% (ANN-3) to 6.72% (PSO-ANN)	Model accuracy drops for Continuous pyrolysis systems, limiting its application at industrial scales.	[140]
Bioethanol production	Establish a data-driven ANN model capable of predicting bioethanol yield in a system	Multilayer Perceptron (MLP) through back propagation.	ANN model demonstrated high predictive accuracy, with reported R^2 values. The model effectively captured strong nonlinear coupling between reaction parameters	Prediction confidence intervals were not reported, limiting industrial applicability. Optimization was conducted solely on yield, without integration of cost, energy efficiency, or emissions	[141]
Hydrogen production	Compared different	Hyper-parameter	PSO-optimized Gradient	A mixed and limited	[142]

	ML models to predict the yield of hydrogen	through Genetic algorithm and PSO	Boosting Regression (Test $R^2 = 0.96$; cross-validation $R^2 = 0.92$). SCWG had more influence on predictions (61%) than feed properties	dataset, with varying experimental conditions, led to underperformance of the ANN model	

Across a wide range of biomass conversion applications, including product synthesis, process kinetics, and feedstock property estimation, machine-learning models consistently outperform simple regression approaches in capturing strongly nonlinear process behavior. Advanced architectures such as ANNs and ensemble methods have shown markedly higher predictive accuracy. This is demonstrated by XGBoost models achieving near-unity coefficients of determination for HHV prediction and by optimization-assisted neural networks substantially reducing kinetic parameter errors. These improvements translate directly into practical benefits, enabling identifying near-optimal operating conditions and reducing experimental runs significantly, while maintaining close agreement with laboratory data. Decision-support frameworks that embed ML within optimization routines demonstrated high ability to guide process exploration efficiently through reporting high prediction accuracy while eliminating a large fraction of trial-and-error experimentation. Despite these advances, important challenges persist in applying AI/ML at commercial levels. Most models are trained on relatively small, laboratory-scale datasets that are often assembled from heterogeneous literature sources, limiting robustness under and reducing transferability of the model to continuous or industrial systems. Moreover, the aggregation of diverse experimental data improves dataset size but also introduces unaccounted variability and uncertainty. Furthermore, uncertainty quantification and confidence interval reporting are largely absent in the present studies, undermining confidence in model predictions for scale-up and investment decisions. Optimization objectives also remain narrowly focused on yield or product distribution, with limited consideration of economic, energy, or environmental performance. Although feedstock screening studies increasingly emphasize interpretable models through feature attribution techniques, many process-level neural network frameworks remain effectively black-box. Overall, the literature reflects a transition from standalone predictive tools toward integrated, decision-oriented artificial intelligence systems, with future progress dependent on improved data quality, uncertainty handling, interpretability, and system-level integration to enable reliable industrial deployment.

The integration of AI and ML into biomass valorization represents a paradigm shift from traditional kinetic theory toward robust, data-driven optimization strategies. Modern applications focus on predictive modeling and advanced characterization. The algorithms of these models bypass classical thermodynamic limitations to accurately forecast product yield, and feed properties based on ultimate and proximate analysis [143,144]. Emerging trends highlight a shift toward sophisticated architecture such as Graph Neural Networks (GNN) for mapping thermal conductivity and Deep Reinforcement Learning (DRL) for autonomous energy management [145]. Furthermore, the adoption of hybrid ML models and spatio-temporal forecasting allows for simultaneous resource assessment and emission reduction. This enables the prediction of biomass availability under fluctuating environmental conditions while correlating feedstock variations directly with combustion outputs [133,135,146]. Despite these advancements, significant opportunities for improvement

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remain, particularly in bridging the gap between laboratory-scale success and industrial implementation [137,147]. Future advancements must prioritize model interpretability through Explainable AI (XAI) to align data-driven insights with underlying physical laws. However, it must be ensured that the standardized, high-frequency experimental databases are fed to the AI models, to improve global model generalizability and reliability across the bioenergy value chain [137].

6. Future Research Opportunities

The production of biofuels has been deeply investigated in this article. However, the limitations of biomass valorization technologies, restrict the use of biomass for energy generation at commercial levels. Besides tackling the elemental issues like high oxygen, nitrogen or sulphur content, there are several other issues, which need to be investigated scientifically, to commercialize biomass conversion techniques. A few of these issues have been identified below, with the intent of providing a research direction for future studies. The aspects are as follows:

a. Design-by-Specification: Setting explicit electronic targets for hydrochar catalysts (like, minimum conductivity, carrier mobility, interfacial electron-transfer rate constants) and use physics-informed models together with operando measurements to backtrack the catalyst synthesis parameters, for achieving the set targets.
b. Metal-Support Electronic Coupling for Hydro-denitrogenation: Engineering bimetallic catalyst systems on electronically tailored hydrochars to promote C-N bond scission in refractory N-species. Further, use operando FTIR and transient methods to resolve rate-limiting steps and inhibition, extending the catalysts lifetime.
c. Interface Engineering in Biphasic Media: Using hydrochar to stabilize Pickering emulsions responsible for co-localizing H_2 activation, acid sites, and electron transfer at water-oil boundaries. Furthermore, application of microfluidics or interfacial spectroscopy could help quantify the coupled mass and charge-transport, suppressing coking or polymerization.
d. Data & AI Integration for Scale-Up: Combining explainable AI with physics-informed neural networks (PNN), and uncertainty quantification can guide experimental selection, while ensuring model reliability beyond lab scale.

7. Conclusions

In summary, biomass valorisation stands as a cornerstone of the global pursuit of carbon neutrality and circular economy strategies. Lignocellulosic residues from agriculture and forestry offer a vast, renewable resource for producing second-generation biofuels and value-added chemicals. While various thermochemical pathways exist, hydrothermal liquefaction (HTL) has emerged as a particularly effective route for processing wet, heterogeneous biomass without the need for pre-treatment of feedstock. The resulting biocrude possesses complex chemical structures that necessitate advanced upgrading techniques, specifically catalytic hydrodeoxygenation. HDO targets the removal of oxygenated compounds from biocrude produced through different thermochemical routes, in presence of hydrogen gas, improving the product quality. Parallel to liquid fuel production, the solid byproduct (hydrochar) demonstrates significant potential as a sustainable energy source (bio-coal), a soil amendment agent for nutrient retention and metal immobilisation, and a versatile support for heterogeneous catalysts. Its physicochemical properties can be further tuned through activation and functionalization to meet specific industrial requirements. Thus, hydrothermal valorization methods help in deriving more than one product from a given feed stock, under specific temperature and pressure conditions. This makes the hydrothermal processes more industry friendly, as compared to other biomass valorization methods. Nevertheless, the TRL scale illustrates that short-term decarbonization will mainly rely on well-established biomass technologies (like pyrolysis, gasification for syngas, torrefication etc.). However, expanding low-carbon fuels in the long term will require further development of less mature technologies, like HTL, and Fischer-Tropsch driven techniques, to make them fully integrated and cost-effective.

Furthermore, the integration of AI and ML represents a vital paradigm shift, enabling the prediction of complex nonlinear relationships in conversion processes. These tools significantly reduce experimental efforts and offer robust decision-support frameworks for process optimization. However, despite these advancements, moving from laboratory-scale success to industrial implementation requires addressing challenges such as catalyst deactivation, nitrogen removal from protein-rich feeds, and model generalizability. Thus, future research must priorities 'design-by-specification' concept for catalyst preparations. Additionally, the use of physics-informed AI could help ensure model reliability during scaling up of these newer technologies. Ultimately, the holistic integration of advanced thermochemical processing with data-driven optimization will be essential for establishing biomass as a reliable and competitive energy carrier in the global energy mix.

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Abbreviations

The following abbreviations are used in this manuscript:

HTL	Hydrothermal Liquification
HTC	Hydrothermal Carbonization
HDO	Hydrodeoxygenation
HDS	Hydro-desulfurization
HDN	Hydro-denitrogenation
AI	Artificial Intelligence
ML	Machine Learning
TRL	Technology Readiness Level

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