Review Article

Bio-Jet Fuel from Vegetable Oils: Production Process and Perspective on Modeling and Simulation

Lida Simasatitkul
Department of Industrial Chemistry, Faculty of Applied Science, King Mongkut's University of Technology North Bangkok, Bangkok, Thailand

Suksun Amornraksa*
Biorefinery and Process Automation Engineering Center, Chemical and Process Engineering Program, The Sirindhorn International Thai-German Graduate School of Engineering (TGGS), King Mongkut's University of Technology North Bangkok, Bangkok, Thailand

Keerthi Katam
Department of Civil Engineering, Ecole Centrale School of Engineering, Mahindra University, Telangana, India

Suttichai Assabumrungrat
Bio-Circular-Green-economy Technology & Engineering Center (BCGeTEC), Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok Thailand
Center of Excellence in Catalysis and Catalytic Reaction Engineering, Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok, Thailand

* Corresponding author. E-mail: suksun.a@tggs.kmutnb.ac.th DOI: 10.14416/j.asep.2024.06.013
Received: 13 February 2024; Revised: 29 March 2024; Accepted: 22 April 2024; Published online: 27 June 2024

Abstract

Bio-jet fuel plays a vital role in mitigating greenhouse gas emissions and reducing the environmental impacts in the air transportation sector. Several production pathways to produce bio-jet fuel have been successfully developed and certified. They can use a variety of materials ranging from edible crops and lignocellulosic biomass to algal oils as feedstock. Various conversion processes can also be used, either thermochemical or biochemical, with and without catalysts. However, among many available processes, producing bio-jet fuel through the hydroprocessed esters and fatty acids (HEFA) route is the most popular. It is also the only route that has so far been commercialized. This review gives an insight into the bio-jet fuel production from vegetable oils, which are the source of HEFA feedstock, with an emphasis on process design and simulation. The use of food and non-food resources as feedstock and the overview of the certified processes for bio-jet fuel production are reviewed and discussed. Additionally, the production process of bio-jet fuel produced from vegetable oils is explored. Finally, the key challenges and prospects of the process simulation and modeling of bio-jet fuel production from vegetable oils are addressed.

Keywords: Aviation fuels standards, Bio-jet fuel production technologies, Hydroprocessed esters and fatty acids (HEFA), Process evaluation, Process simulation and modeling

1 Introduction

The air transport demand is recovering rapidly and will continue to grow steadily, leading to increased aviation emissions [1]. The global consumption of aviation fuel is anticipated to increase from 106 billion gallons in 2019 to 230 billion gallons in 2050 [2]. Traditional jet fuel combustion yields approximately 3.2 kg of CO_2 per kg of jet fuel burned, significantly contributing to greenhouse gas (GHG) emissions. The aviation sector is estimated to account for approximately 2.5% of energy use-related CO_2 emissions [3]. However, research demonstrates that using aviation fuel derived from hydrogenated vegetable oils and Fischer-Tropsch synthesis (FT) can reduce greenhouse gas emissions by 70–90% compared to petroleum-derived jet fuel under specific conditions [4]. In response to global climate change concerns, bio-jet fuel, or sustainable aviation fuel (SAF), has garnered significant attention over the past decade. Bio-jet fuel, produced from renewable resources such as biomass, agricultural residuals, and vegetable oils, exhibits physicochemical properties equivalent to petroleum-based jet fuel, ensuring seamless substitution [5].

In response to the potential of bio-jet fuel in mitigating greenhouse gas emissions, various air transport policies and regulations have been instituted to promote its increased usage. Notably, the International Organization of Air Transport (IATA) set a target in 2009 to halve CO_2 emissions by 2050 [6]. Initiatives like the RefuelEU aviation initiative from the European Council aim to reduce net greenhouse gas emissions by at least 55% by 2030 and attain climate neutrality in 2050, mandating fuel suppliers to incorporate 2% SAF in 2025, 6% in 2030, and 70% in 2050 [7]. The Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA), mandated by the International Civil Aviation Organization (ICAO), necessitates a substantial reduction in CO_2 emissions from 2021 to 2035, underscoring the imperative of SAF utilization [8]. Consequently, an increased demand for bio-jet fuel is anticipated, underscoring the pivotal role of research and development in bio-jet fuel production.

Jet fuel, conventionally derived from crude oil, undergoes distillation at temperatures ranging from 205 to 260 °C. The resulting distillates, encompassing carbon numbers C_8 to C_{16}, consist of linear, branched chain, cyclic, and aromatic compounds [9], [10]. Alkanes serve as the primary energy source for aircraft engines, while iso-alkanes enhance cold flow properties and energy content. Naphthene is employed to lower the freezing point, and the presence of aromatics contributes to fuel lubrication and aids in preventing leaks in airplane seals. Adherence to standard fuel properties, including energy density, flash point, freezing point, density, viscosity, aromatic content, sulfur content, and conductivity, is imperative for jet fuels. Two widely accepted international jet fuel specifications are ASTM D1655 (Standard Specification for Aviation Turbine Fuels), certified by ASTM International, and DEF STAN 91-91 (Turbine Fuel, Aviation Kerosene Type, Jet A-1), a standard specified by UK Ministry of Defence. These specifications, and others, are all very similar, having nearly identical requirements.

Jet fuels are categorized into commercial (Jet A-1, Jet A, Jet B) and military (JP-4, JP-8) fuels, with Jet A-1 being the most widely used commercial jet fuel and a representative of jet fuels [11], [12]. The military fuels are the same as the commercial jet fuels but contain additional additives such as corrosion and icing inhibitors. Jet A, typically used in the US and Canada, has a slightly higher freezing point than Jet A-1, while Jet B, having a maximum freezing point of –50 °C, is only used in extreme cold conditions. It should be noted that the ASTM D1655 serves as a standard for petroleum-based jet fuel. If the jet fuel is to be produced from renewable resources, it must comply with the batch specification of ASTM D7566 (Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons), and the final fuel properties when blended with petroleum-based Jet A-1 must comply with the ASTM D1655 jet-fuel standard. A comparison of aviation fuel specifications of ASTM D7566, ASTM D1655, and IATA standards is presented in Table 1 [13]–[16].

Bio-jet fuel, reported to be economically and technologically advantageous, can be produced from a diverse array of renewable feedstocks [17]. While numerous feedstocks and conversion pathways have been certified by ASTM for bio-jet fuel production, the hydroprocessed esters and fatty acids (HEFA) route is the sole commercially available pathway, powering more than 95% of all SAF flights today [18]. Despite comprehensive reviews on bio-jet fuel production, focusing on process technology, feedstock comparisons, catalyst developments, environmental consequences, and techno-economic aspects, the modeling and simulation of the HEFA process have received limited attention. This review addresses this gap, providing insights into the modeling and simulation of bio-jet fuel production from vegetable oils. It elucidates the types of feedstocks, the latest certified production pathway, and critically examines progress, challenges, and future perspectives in the modeling and simulation of the HEFA process.

Table 1: Specifications of conventional jet fuels and alternative jet fuel

Properties	ASTM D7566 (HEFA)	ASTM D1655	DEF STAN 91-91
Higher heating values (MJ/kg) Min.	42.8	42.8	42.8
Viscosity (mm^2/s) at –20 °C Max.	8.0	8.0	8.0
Density (kg/m^3) at 15 °C	730–772	775–840	775–840
Flash point (°C) Min	38	38	38
Freezing point (°C) Max	–40	–47	–47
Final BP (°C)	300	300	300
Total acidity (mg KOH/g)	0.1	0.1	0.015
Aromatics (wt%) Max.	25	25	25
Smoke point (mm) Min.	25	25	25
S (mass %) Max.	0.3	0.3	0.3
Conductivity (pS/m)	50–600	50–450	50–600

2 Feedstock for Bio-Jet Production

Bio-jet fuel, derived from biofuels, can be produced from various feedstocks, including edible and non-edible crops, animal fats, lignocellulose, and algae. First-generation biofuels, produced from edible crops, primarily rely on simple sugars from food crops like sugarcane and starches (corn, wheat, or cassava starch) through fermentation processes, yielding bioethanol which is used as a gasoline substitute. Biodiesel, another major first-generation biofuel, is derived commercially from food crops containing vegetable oil, such as soybeans, palm, canola, and rapeseed, through transesterification. These feedstocks are very common and abundantly available in many regions. For example, the growth of oil palm plantations can be enough to serve biodiesel production [19]. Despite the well-established technology for first-generation biofuels, as evidenced by numerous commercial-scale plants operating worldwide, their use of edible feedstocks exacerbates the food versus fuel conflict, presenting challenges in supply-demand balancing, water management, and land use [20]. Second-generation and third-generation biofuels have been explored and developed to address these challenges. The comparison of the production of first-generation, second-generation, and third-generation biofuels is illustrated in Figure 1.

Second-generation biofuels are produced from non-edible crops, lignocellulose, and animal feedstocks, including agricultural and forest residues, food waste, and specific energy plants. Agricultural residue, comprising leftover plant material, represents a promising lignocellulosic material for biofuel production due to its abundant global production. It is estimated that about 1.5–3.9 billion tonnes of agricultural residue is generated globally each year [21], [22]. However, despite being a waste product, the cost of agricultural residue is not negligible, primarily due to material gathering and transportation expenses. The bulky and lightweight nature of most residues necessitates a large volume for operating a commercial-scale plant, resulting in high transportation costs. Additionally, the availability of residue may be limited as it is often utilized as a low-grade fuel for energy production on small and large scales [23]. With an estimated 600 million tonnes generated annually, food waste emerges as a potential feedstock source for biofuel production [24]–[26]. Due to its high fermentable material content, food waste is relatively more straightforward to be converted into biofuel through anaerobic digestion [27], [28]. However, if food waste is to be utilized for producing aviation biofuels, it must compete in both the power generation and alternative liquid fuel sectors.

Specific energy plants with high lignin and cellulose content, such as perennial grasses (e.g., switchgrass and Napier grass) and short rotation forestry crops (e.g., willow or poplar) offer alternative lignocellulosic feedstocks with low fertilizer-input requirements, low energy cultivation, and suitability for marginal land [29]. Lignocellulosic biofuels provide a substantial reduction in greenhouse gas emissions. They utilize

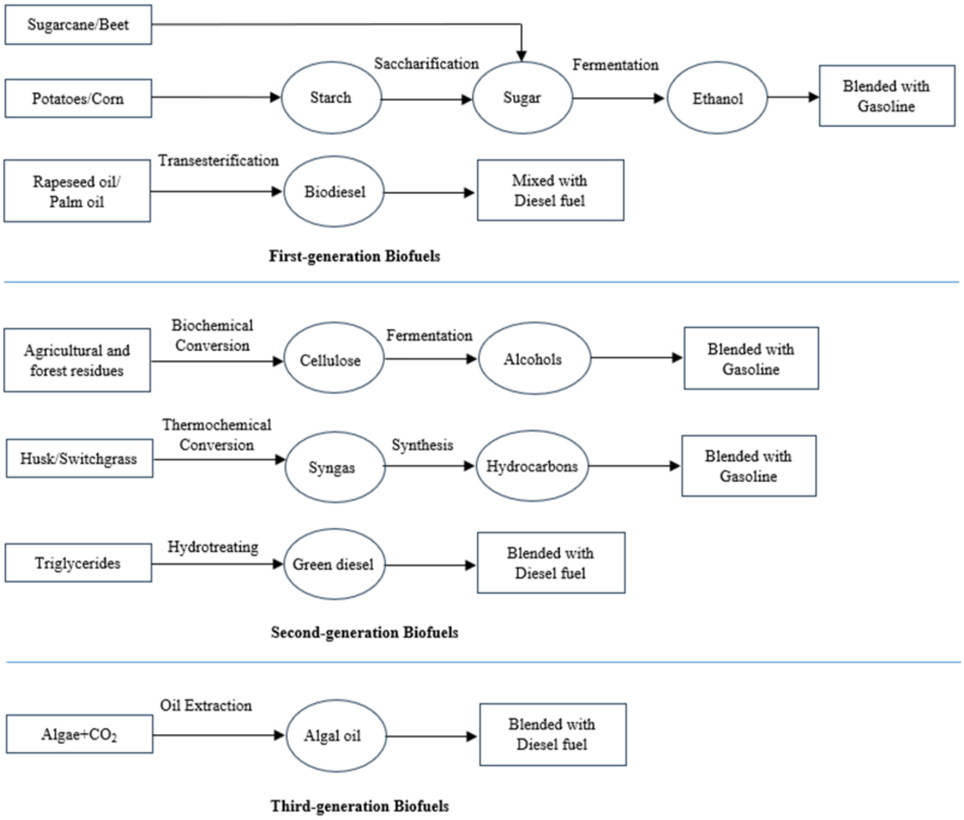

Figure 1: Production of first-generation, second-generation, and third-generation biofuels.

abundant and low-cost non-edible feedstocks, thus avoiding interference with the human food chain [30]. Moreover, they can be tailored to meet petroleum-derived jet fuel specifications [31]. However, a large-scale plant required to produce commercial lignocellulosic biofuels is capital-intensive, resulting in comparatively high fuel costs. Furthermore, there are associated risks, such as the security of feedstock supply and fluctuating oil prices, making commercialization challenging without government support.

Triglycerides derived from non-food plants, waste vegetable oils, and algae offer alternatives to lignocellulosic feedstocks without the food competition issue. These feedstocks can either be used to produce biodiesel through a conventional transesterification process or be converted into hydrocarbons through a hydrodeoxygenation reaction. Examples of non-food plants that can be used as triglyceride sources include Jatropha, Karanja, castor, camelina, and linseed. Among them, jatropha is the leading cultivated plant, generating more oil than other plants [32]. Jatropha is grown in many countries, especially in India, Africa, and similar climates. It can also be grown all the year [33]. Camelina is easy to grow and can produce a large amount of oil seeds. It can grow well in hot climates. Every year, 800 million metric gallons of oil are produced from camelina [34]. Waste cooking oils (WCO) serve as a substantial source of triglycerides for biodiesel production, with an estimated 25 million tonnes available globally [35]. However, the use of waste cooking oil as a biodiesel feedstock requires significant pretreatment due to elevated levels of free fatty acids, water, and solid impurities [36].

Third-generation biofuels are derived from algal feedstock. Some microalgae species can absorb CO_2 from the air to multiply and produce a lot of oils, which can be extracted and used directly as a biofuel. This biofuel production method is attractive as the CO_2 from the air can be captured and converted into biofuels directly, without going through several conversion steps like the second-generation biofuels [37]. The lipid composition of microalgae varies based on many factors, such as species and culture conditions, offering diverse possibilities for biofuel production [38]. For example, some strains of Chlorella vulgaris can produce C_6 chains, while the halophyte Isochrysis galbana produces longer chains of up to C_{24}. Marine species, such as strains of Chlorella salina, can produce C_{22} unsaturated esters with up to six double bonds [39]. Algal-derived biofuels have gained much interest as a sustainable biofuel [40]. However, despite extensive research, no commercial plant has emerged until now. The main reason is due to the non-competitive cost of lipid production from microalgae [41].

3 Production Processes of Bio-Jet Fuel

The aviation industry mandates the exclusive use of a designated jet fuel, Jet A-1, for optimal turbine and engine performance. Various bio-jet fuel production pathways have been systematically developed to comply with industry standards and attain certification from the American Society for Testing and Materials (ASTM). These pathways encompass the Fischer-Tropsch-to-jet, hydroprocessed esters and fatty acids (HEFA) or Oil-to-jet, sugar-to-jet, and alcohol-to-jet processes [42]. As of the current date, ASTM has certified eleven distinct conversion processes for bio-jet fuel, as delineated in Table 2 [43]–[46].

The first certification in 2009 was conferred upon the Fischer-Tropsch (F-T)-to-jet process, which entails the conversion of lignocellulosic feedstocks, including biomass and municipal solid waste (MSW), as well as non-renewable feedstocks like coal and natural gas [47]. This process involves the transformation of these feedstocks into a synthesis gas (i.e., a mixture of carbon monoxide and hydrogen). After purification, the purified synthesis gas is converted into long carbon chain waxes through Fischer-Tropsch (F-T) synthesis. The resultant wax undergoes cracking and isomerization to yield drop-in liquid fuels akin to the paraffinic kerosene present in traditional petroleum-based jet fuel.

Table 2: ASTM-certified conversion processes for bio-jet fuel production

Abbreviation	Conversion Process	Feed	Blend Limit	Developer
FT-SPK	Fischer-Tropsch to synthetic paraffinic kerosene	Coal, natural gas, biomass	50%	Sasol, Shell, Fulcrum Bioenergy, Syntroleum
HEFA-SPK	Hydroprocessing of esters and fatty acids to synthetic paraffinic kerosene	Bio-oils, animal fat, recycled oils	50%	Honeywell, UOP, Neste, Dynamic Fuels, EERC
HFS-SIP	Hydroprocessing of fermented sugars to synthetic iso-paraffins	Biomass used for sugar production	10%	Total, Amyris
FT-SKA	Synthetic kerosene with aromatics derived by alkylation of light aromatics from non-petroleum sources	Coal, natural gas, biomass	50%	Sasol, Shell
ATJ-SPK	Alcohol to synthetic jet paraffinic kerosene	Ethanol, i-butanol or isobutene from biomass	50%	Gevo, Lanzatech, Byogy
CHJ	Catalytic hydrothermolysis to jet fuel	Triglycerides such as soybean oil and jatropha oil	50%	Applied Research Associates
HC-HEFA-SPK	Hydrocarbons-HEFA to synthetic paraffinic kerosene	FOGs, Algae	10%	N.A.
ATJ-SKA	Alcohol to synthetic jet paraffinic kerosene with aromatics	Mixed C2-C5 alcohols derived from a mixture of CO_2 and H_2	50%	Swedish Biofuels
Co-processed HEFA	Co-hydroprocessing of esters and fatty acids in a conventional petroleum refinery	Fats, oils, and greases (FOG) co-processed with petroleum	5%	Chevron, Phillips66, BP
Co-processed FT	Co-hydroprocessing of Fischer-Tropsch hydrocarbons in a conventional petroleum refinery	FT hydrocarbons co-processed with petroleum	5%	N.A.
Co-processed biomass	Co-hydroprocessing of biomass	Biomass-derived hydrocarbons co-processed with petroleum	5%	N.A.

Note: Blend limit means the maximum allowable blending ratio of the synthesis fuel in the aviation fuel.

Hydroprocessed Esters and Fatty Acids (HEFA)-to-jet process, certified in 2011, employs vegetable oils, waste oils, or fats as feedstock [48]. These feedstocks are subjected to hydrotreating, a process involving hydrogen treatment to eliminate oxygen and undesirable molecules. The resultant straight paraffinic hydrocarbons undergo cracking and isomerization, forming a synthetic jet fuel component predominantly composed of paraffinic kerosene.

Hydroprocessed Fermented Sugars (HFS), or sugar-to-jet, process, certified in 2014, represents the sole bio-jet fuel production process based on a biochemical platform [49]. This method utilizes modified yeasts and microbes to ferment C_6 sugars into farnesene, a C_{15} hydrocarbon molecule. Notably, due to the resulting paraffin's singular carbon chain length, its certified blending ratio with petroleum-derived jet fuel is capped at 10%, in contrast to the 50% allowance for other certified processes.

Synthetic Kerosene with Aromatics (FT-SKA), certified in 2015, combines the F-T Synthesis Process with the alkylation of light aromatics, primarily benzene. This amalgamation produces a hydrocarbon blend with aromatic compounds crucial for ensuring elastomer seal swell in aircraft components, thereby preventing fuel leaks. FT-SPK/A signifies a shift toward fuels encompassing a full spectrum of molecules found in petroleum-based jet fuel, as opposed to exclusive paraffin [6].

Alcohol-to-jet (ATJ-SPK) process, certified in 2016, employs ethanol and iso-butanol as feedstock, sourced either from the fermentation of starches/sugars or derived from cellulosic biomass. The alcohols undergo dehydration, oligomerization, hydrogenation, and fractionation, resulting in hydrocarbons with the desired carbon chain length.

Catalytic hydrothermolysis to jet fuel (CHJ), certified in 2020, is similar to the HEFA-to-jet in that it can utilize various triglycerides from plants, animal fats, oils, and greases as feedstock. The fatty acid esters and free fatty acids undergo catalytic hydrothermal conversion, combined with hydrotreating, hydrocracking, or isomerization. The treated products containing paraffinic, iso-paraffinic, cyclo-paraffinic, and aromatic compounds are subsequently fractionated to isolate the synthetic jet fuel [50].

Catalytic hydrothermolysis to jet fuel (CHJ), certified in 2020, is similar to the HEFA-to-jet in that it can utilize various triglycerides from plants, animal fats, oils, and greases as feedstock. The fatty acid esters and free fatty acids undergo catalytic hydrothermal conversion, combined with hydrotreating, hydrocracking, or isomerization. The treated products containing paraffinic, iso-paraffinic, cyclo-paraffinic, and aromatic compounds are subsequently fractionated to isolate the synthetic jet fuel.

Hydrocarbons, Hydroprocessed Esters and Fatty Acids (HC-HEFA), also certified in 2020, mirrors the HEFA process, using bio-derived hydrocarbons, free fatty acids, and fatty acid esters. Hydroprocessing transforms these components into saturated hydrocarbons, eliminating all oxygen content. Notably, this is the sole certified process capable of utilizing algae, such as Botryococcus braunii species, as the feedstock.

The most recent addition to the certified bio-jet fuels pathways, Alcohol-to-jet Synthetic Paraffinic Kerosene with Aromatics (ATJ-SKA), received certification in 2023. This process employs a combination of C_2–C_5 alcohols as feedstock, allowing for the production of biofuel containing a small percentage of aromatic hydrocarbons essential for optimal jet fuel performance. The C_2–C_5 alcohols used in the process can be derived from the fermentation of starches/sugars sourced from both first- and second-generation feedstocks. Additionally, biogas and a mixture of carbon dioxide and hydrogen can serve as alternative sources for producing these alcohols.

Conversely, the co-hydroprocessing of HEFA, FT, and biomass pathways involves the integration of bio-oils obtained from HEFA, Fischer-Tropsch, or biomass - up to 5% by volume - into existing petroleum refinery processes. Despite the certification of these pathways as bio-jet fuel production methods, they are not recognized as sustainable practices. This is primarily attributable to the utilization of raw materials within these co-hydroprocessing pathways, which, regrettably, remain predominantly sourced from fossil fuels.

A noteworthy observation relates to the diverse blending limits imposed on bio-jet fuel obtained from certified conversion pathways when combined with Jet A-1 fuel. The maximum allowable blending ratio stands at 50%. This limitation stems from the predominant composition of paraffins and iso-paraffins in the synthesized bio-jet fuel, lacking the requisite

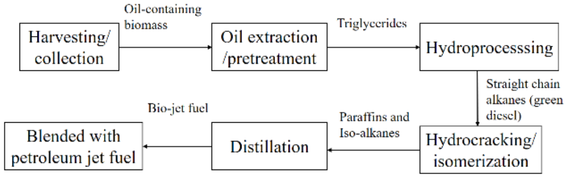

Figure 2: Process of HEFA bio-jet fuel production.

content of cyclic and aromatic compounds found in conventional jet fuels. Consequently, the distinctive properties of bio-jet fuel hinder its ability to achieve a complete replacement of traditional jet fuels [51].

4 Production of Bio-Jet Fuel from Vegetable Oil

As previously noted, the HEFA-to-oil pathway stands out as the most advanced and only commercial process for producing bio-jet fuel. This section furnishes the scientific community with a comprehensive overview and process description of the HEFA process, serving as a foundational resource for an enhanced grasp of the modeling and simulation intricacies intrinsic to the HEFA process. Developed by UOP Honeywell, the HEFA process entails the conversion of vegetable oil feedstock into paraffinic hydrocarbons featuring 9–16 carbon atoms and a notably high iso/normal ratio, rendering them suitable for aviation fuel applications [52]. Figure 2 encapsulates a summarized and illustrative depiction of the HEFA bio-jet fuel production process.

Primarily, the essence of the HEFA bio-jet fuel production revolves around two pivotal conversion steps—hydroprocessing and hydrocracking coupled with isomerization (a two-step process). Hydroprocessing, or hydrotreating, constitutes a crucial phase intended to remove the oxygen content and other undesirable impurities inherent in the triglyceride feedstock. During the hydroprocessing, which generally occurs at a temperature range between 300–350 °C, a combination of hydrodeoxygenation (HDO), decarbonylation (DCO), and decarboxylation (DCO_2) reactions simultaneously take place [53]. The HDO reaction uses a large amount of hydrogen to crack the triglycerides and convert the oxygen in the oils into water. On the other hand, the DCO_2 uses a small amount of hydrogen to remove carboxyl groups from the oils and convert them into CO_2 gas. Compared to both reactions, the DCO uses a medium amount of hydrogen to remove the carboxyl groups, converting them into CO and water [54]. In any case, shorter straight-chain alkanes and propane are obtained as a product and by-product of the reactions. For elucidation, considering palmitic triglyceride as a model, the equations for the hydrodeoxygenation (HDO), decarboxylation (DCO_2), and decarbonylation (DCO) reactions are articulated as follows [55].

Hydrodeoxygenation (HDO):

$$C_{51}H_{98}O_6 + 12H_2 \rightarrow 3C_{16}H_{34} + C_3H_8 + 6H_2O \qquad (1)$$

Decarboxylation (DCO_2):

$$C_{51}H_{98}O_6 + 3H_2 \rightarrow 3C_{15}H_{32} + C_3H_8 + 3CO_2 \qquad (2)$$

Decarbonylation (DCO):

$$C_{51}H_{98}O_6 + 6H_2 \rightarrow 3C_{15}H_{32} + C_3H_8 + 3CO + 3H_2O \quad (3)$$

The hydroprocessed product derived from the reactor consists of straight-chain alkanes comprising 15–18 carbon atoms, accompanied by propane, CO, CO_2, and water as by-products. These extended-chain alkanes, recognized as bio-hydrogenated diesel (BHD) or green diesel, have been considered premium diesel due to their superior heating value, high cetane number, and low sulfur content in comparison to biodiesel produced through transesterification [56], [57]. Notably, despite the hydrogen efficiency of DCO_2 and DCO being higher than that of HDO, these processes entail a carbon loss and subsequent energy content reduction [58]. Moreover, CO and CO_2 are deemed less favorable due to their contribution to carbon emissions, with the potential to undergo methanation reactions, consuming a substantial amount of hydrogen. Consequently, HDO technology is considered a more efficient pathway than DCO and DCO_2 [59].

The hydroprocessing reactions are typically facilitated by metal catalysts imbued with hydrogenation functionality, such as Pt, Pd, Pt-Re, or sulfide NiW, CoMo, and NiMo, supported over nonacidic substrates like activated carbon, zeolites, or oxides [60]. Nevertheless, it is imperative to acknowledge that hydroprocessing alone does not directly yield optimal quantities of bio-jet fuel. Although mild hydrocracking may occur amid HDO, DCO_2, and DCO reactions, controlling the extent of cracking is impractical owing to the non-alignment of reaction temperature, pressure, and catalyst specifications for this purpose. Furthermore, undesirable fractions of short-chain alkanes (C_1–C_6) can be produced under inappropriate cracking conditions [61]. Consequently, a secondary reactor engineered specifically for cracking and isomerization becomes indispensable to amass a substantial yield of bio-jet fuel, predominantly C_8–C_{15} hydrocarbons.

Cracking and isomerization processes typically unfold within a temperature range of 350–450 °C, generating bio-jet fuel with a substantial yield of iso-alkanes [12]. Generally, the cracking step truncates heavy hydrocarbons into lighter unsaturated hydrocarbons. Hydrocracking—cracking in the presence of hydrogen and a catalyst—is conventionally employed due to the need for saturated hydrocarbons. To keep the freezing point of bio-jet fuel lower, a significant fraction of iso-alkane in the fuel is imperative [62]. Therefore, the isomerization step, which transforms linear hydrocarbons into branched hydrocarbons, is indispensable in bio-jet fuel production [63]. Acidic catalysts, including noble metals, sulfonated metals, oxides, and bimetallic materials are typically used in both processes [64]. Common catalysts used for hydrocracking and isomerization reactions include Ni, Pt, and other precious metals. The catalyst supports include activated carbon, Al_2O_3, and zeolite [42]. The temperature and pressure parameters for the cracking process are contingent upon the type of catalyst employed, ranging from 360–450 °C and 40–130 bar for sulfided catalysts to 270–300 °C and 30–55 bar for Ni and Pt metal-based catalysts [65].

A wealth of literature has delved into the realm of bio-jet fuel production. Lin *et al.* [16] studied bio-jet fuel production by using crude palm oil as a feedstock in the presence of NiMo-S/γ-Al_2O_3 as a catalyst. The optimal conditions are the reaction temperature of 360 °C, the pressure of 3 MPa, and the hydrogen/oil molar ratio of 13.6. The viability of Jatropha curcas oil as a renewable raw material for bio-jet production was explored by Gutiérrez-Antonio *et al.* [66]. The impact of operating parameters such as reaction temperature, pressure, amounts of catalysts, and hydrogen flow rate were investigated for bio-jet production from crude palm kernel oil [67]. Vásquez *et al.* [59] summarized the reaction pathways and yield of hydroprocessing of vegetable oils under various conditions. Khan *et al.* [62] reviewed the deoxygenation and hydrodeoxygenation reaction pathways and mechanism of model compounds (i.e., methyl esters, triglycerides, vegetable oils). Chehadel *et al.* [68] gathered kinetic modeling of heavy oil and residue. Wei *et al.* [42] reviewed bio-jet production from diverse feedstocks.

The following sections will provide a comprehensive review of the computer-aided design for bio-jet fuel production from vegetable oils to expand our understanding. The first section will focus on using the computational fluid dynamic (CFD) technique to aid in designing the hydroprocessing reactors. The second section involves the process design on a commercial scale using process simulators. Both segments encapsulate a trifold perspective encompassing technology, economics, and the environment. Finally, advancements in simulations utilizing machine learning for bio-jet production are also elucidated.

4.1 *Process design of bio-jet production*

4.1.1 Process simulation

Modeling and simulation play pivotal roles in expediting research endeavors while mitigating time and cost considerations. Mathematical models, incorporating mass balance of components, energy balance, momentum balance, thermodynamic relations, and chemical kinetics, serve as the foundation. Computational fluid dynamics (CFD), a numerical analysis technique, facilitates the resolution of fluid flow intricacies and distribution. The formulation of mathematical models involves partial differential equations (PDEs), boundary conditions, mesh design, initial coordinates, and time considerations. These principles find application in modeling reactor equipment. Literature reviews relate to the hydroprocessing of vegetable oil for bio-hydrogenated diesel and hydrocracking for bio-jet fuel, employing CFD. The critical information are kinetic rates, catalyst properties, and chemical properties of components.

The PDEs consist of the continuity equation, momentum conservation, standard k-epsilon turbulent model (k–ε), and energy conservation as shown in Equations (4)–(8). The co-ordinate of equations depends on geometry reactor such as cylindrical co-ordinate.

Continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla(\partial \bar{u}) = 0 \tag{4}$$

Momentum conservation

$$\rho\left(\frac{\partial \vec{u}}{\partial t}+\vec{u}\cdot\nabla\vec{u}\right)=-\nabla p+\mu\nabla^{2}\vec{u}+\rho\vec{g} \tag{5}$$

Standard *k*-epsilon turbulent model (*k*–ε)
For turbulent kinetic energy

$$\frac{\partial\rho}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] +G_k+G_b-\rho\varepsilon-Y_M \tag{6}$$

For dissipation

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_i}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right] +C_{1\varepsilon}\frac{\varepsilon}{k}(P_k+C_{3\varepsilon}P_b)-C_{2\varepsilon}\rho\frac{\varepsilon^{2}}{k}+S_\varepsilon \tag{7}$$

Energy conservation

$$\begin{aligned}\rho(\rho E)&=-\nabla\cdot\left(\vec{u}(\rho E)\right)-(\vec{u}q)+\rho(\vec{u}\cdot g)\\&=-\nabla\cdot(p\vec{u})-\left(\vec{u}[\vec{\tau}\cdot u]\right)+S_h\end{aligned} \tag{8}$$

The mesh design is important for CFD because it is applied to the numerical calculation. For geometry in 2 dimensions, triangle and rectangular can be used to generate grids. While tetrahedral, hexahedral are used for 3 dimensions. The mesh quality depends on mesh geometry and size. Small meshes perform more accurate solutions but require large disk space.

The boundary condition of a hydrotreating reactor relates to the operating conditions. For example, liquid inlet condition, gas inlet condition, outlet condition for products, no slip wall are defined. The example of boundary conditions for fluid flow is [69]

At $t = 0$, $u_z = 0$ for $0 \le r \le R$
At $r = 0$, u_z = finite
At $r = R$, $u_z = 0$

The example of boundary conditions for mass transfer is

At $z = 0$, $u_{H2} = 0$
At $z = L$, $\frac{\partial C_i}{\partial z} = 0$
At $r = 0$, $\frac{\partial C_i}{\partial r} = 0$

Furthermore, boundary condition can be added at the interface between liquid phase and gas phase by Henry's law.

Atthanatho [69] proposed a kinetic model of hydrotreating of Jatropha oil with $NiMo/Al_2O_3$ catalyst when the Langmuir-Hinshelwood was presented as a kinetic model. The multiphase chemical flow model in a microchannel reactor was developed using COMSOL Multiphysics software. This modeling consisted of a gas-liquid slug flow system for mass transfer, heat transfer, and chemical reactions. The bubble formation mechanism in the microchannel and velocity profile of the liquid slug were performed with different residence times. Their results indicated the successful formation of hydrocarbon C_{17}–C_{18}, fatty acids, and fatty alcohols under a specific temperature of 325 °C, pressure of 500 psig, and residence time of 37 s.

A study on hydrotreating of non-edible vegetable oil in a vertical cylindrical trickle bed reactor using $NiMoP/Al_2O_3$ as a catalyst was conducted. A two-dimensional axisymmetric model was used to simulate the reactor to illustrate the concentration distribution of hydrocarbon C_{17} and C_{18} in liquid and solid phases. performed. The reactor diameter is 1.5 m while its length is 8 m. Optimal conditions resulted in 88.3% conversion of triglyceride, yielding 58.5% renewable diesel at an inlet temperature of 375 °C [70].

The hydrodeoxygenation of bio-oil in a two-dimensional ebullated bed reactor was modeled by CFD. The reaction temperature from 350–400 °C was studied. The mass fractions of heavy non-volatile compounds, light volatile compounds, alkanes, aromatics, hydrogen, water, and coke were performed [71]. Generally, NiMo catalyst was used as a catalyst to produce aliphatic alkanes. Aromatic compounds were observed when a Mo/Al_2O_3 catalyst was employed. Another study simulated the hydrodeoxygenation of Pine pyrolytic oil in a fixed bed reactor in the presence of Pt/Al_2O_3, revealing the presence of alkanes and aromatics with an increase in weight hourly space velocity (WHSV) [72].

Tirado *et al.* [73] proposed kinetic modeling of hydrotreating vegetable oil to produce hydrocarbons across different molecular weights ranging from heavy hydrocarbons (C_{15}–C_{18}), middle hydrocarbon

(C_9–C_{14}), and light hydrocarbon (C_5–C_8), with a NiW/SiO_2–Al_2O_3 catalyst. The CFD modeling spanned small-scale and large-scale trickle bed reactors, presenting production yields along the catalyst bed length. Complete triglyceride conversion occurred at the halfway mark of the reactor, emphasizing the significance of temperature profiles for different hydrocarbon yields.

Muharam *et al.* [74] simulated the hydrocracking of vegetable oil by using a NiW/SiO_2 catalyst. The hydrocarbon products obtained were divided into four categories, i.e., naphtha (C_3H_8, C_6H_{14}, and C_8H_{18}), kerosene (C_9H_{20} and $C_{11}H_{24}$), diesel ($C_{17}H_{36}$), and wax ($C_{19}H_{40}$). A two-dimensional axisymmetric model was used to simulate a slurry bubble column reactor using CFD. The triglyceride and hydrogen flow were in an upward direction. The product concentration profiles were performed in the liquid phase and gas phase. The results showed that the catalyst distribution at the bottom was more concentrated due to the gravity force. Optimal conditions resulted in a 99.26% triglyceride conversion, a 40.68% w/w product yield, and 45.55% w/w purity.

Quiroz-Pérez *et al.* [75] focused on modeling a non-isothermal liquid-vapor flow for bio-jet production. The reactions were hydrodeoxygenation, cracking, and isomerization, and C_8–C_{16} hydrocarbons were produced. The study analyzed the geometry of tray design, including tray spacing, hole diameter, weir height, clearance under the downcomer, and downcomer area, and its impact on liquid volume fraction in two dimensions. The Eulerian approach in the Governing equations, the momentum and heat transfer interface, was applied to analyze the hydrodynamic effects.

It is evident that critical data for CFD simulations derive from kinetic models derived from experimental data. CFD simulations, though, currently face limitations at the macro-scale. The exploration of catalyst structures at the micro-scale, such as foam catalysts, remains challenging due to the absence of heterogeneous reaction kinetic rates. A detailed overview of the CFD model for hydroprocessing is presented in Table 3.

The process design of bio-jet production is modeled through process simulation software, such as Super Pro Designer and Aspen Plus. Using process simulation software to design and optimize a process has become a prevailing practice today, owing to its capacity to substantially reduce the time consumption for evaluating process feasibility. Steady-state assumptions underpin the generation of process flowsheets, wherein mass and energy balances are modeled through unit operations within Aspen Plus forms. Due to the intricacies of triglyceride structures, simplified triglycerides such as trilaurin, trimyristin, tripalmitin, and triolein are used as model compounds [76]. The incorporation of a thermodynamic equation model becomes imperative for predicting vapor-liquid equilibrium and missing properties. Researchers

Table 3: CFD models of the hydroprocessing processes

Reaction Process	Reactor	Modeling	Software	Ref.
Hydrotreating of vegetable oil	Microreactor	Mass balance: gas-liquid slug flow system Kinetic model: Langmuir-Hinshelwood	Comsol Multiphysics	[69]
Hydrotreating of non-edible vegetable oil	Trickle bed reactor	Momentum balance: two-phase Darcy’s law Mass balance: convection-diffusion for gas and liquid phase Kinetic model: Langmuir-Hinshelwood	Comsol Multiphysics	[70]
Hydrodeoxygenation of bio-oil	ebullated bed reactor	Heat balance: Turbulent kinetic energy for multiphase	ANSYS Fluent	[71]
Hydrodeoxygenation of Pine pyrolytic oil	Fixed bed reactor	Momentum balance: Eulerian multiphase turbulence model Kinetic model: Lump model	ANSYS Fluent	[72]
Hydrotreating of Jatropha oil	Trickle bed reactor	Mass balance: neglect plug flow deviation or hydrodynamic effects Energy balance: non-isothermal Kinetic model: Lump kinetic model	Comsol Multiphysics	[73]
Hydrotreating of Jatropha oil	Slurry bubble column reactor	Mass balance: dispersion-convection Heat balance: convection-conduction model Kinetic model: Lump kinetic model	Comsol Multiphysics	[74]
	Reactive distillation	Momentum transfer: K-epsilon ($\kappa - \varepsilon$) turbulence model Kinetic model: Lump kinetic model	ANSYS Fluent	[75]

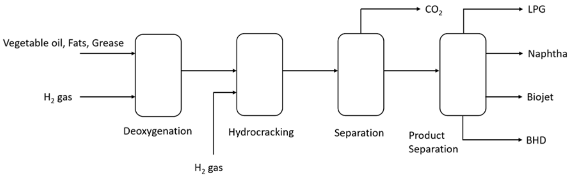

Figure 3: UOP Green jet fuel production process.

commonly undertake the comprehensive design of the bio-jet production process, including optimization of process parameters and heat integration. The kinetic models are usually not employed due to the lack of required kinetic data. Conversion reactor [52], [77], [78] and yield reactor [79] models are frequently used instead. Various aspects of the design objectives are usually considered, including the maximization of product yield, economic viability, and environmental impacts. For the bio-jet production from vegetable oils, most of the process flowsheets originated from the UOP Green jet fuel production process, which can produce multiple products such as LPG, naphtha, bio-jet fuel, and BHD, as shown in Figure 3 [80].

The hydrotreating of vegetable oil initiates the generation of fatty acids, bio-hydrogenated diesel (BHD), propane, and CO_2. Subsequent steps involve the isomerization and cracking of BHD, resulting in light hydrocarbons (C_3–C_7), bio-jet fuel (C_8–C_{16}), and BHD (C_{17} and C_{18}) [52]. Various studies, such as Martinez-Hernandez *et al.* [81], have outlined detailed process flowsheets encompassing hydrotreating reactions, isomerization reactions, dewatering, hydrogen recovery, and distillation columns for naphtha, bio-jet fuel, and BHD purification, as shown in Figure 4.

The hydrotreating process can be achieved in one reactor, including hydrodeoxygenation, hydrocracking, and isomerization. However, this process simulation method requires a complete hydrolysis of vegetable oil to form fatty acids before the hydrotreating [82].

While the standalone bio-jet fuel production process is commonly used, combining esterification and hydrotreating of waste cooking oil was proposed [83]. This process allowed the production of renewable products such as biodiesel, glycerol, naphtha, bio-jet, and BHD. The heat integration was considered when the conventional bio-jet production process was designed entirely. Gutiérrez-Antonio *et al.* [84] proposed a conventional bio-jet production process including direct sequence and indirect sequence of distillation columns to separate light hydrocarbons, bio-jet fuel, and BHD. Then, the thermally coupled distillation sequence, thermal direct coupled column, thermal indirect coupled column, petlyuk column, and divided wall column were analyzed.

The results revealed that the thermal direct coupled column and thermal indirect coupled column offered the minimum energy consumption and minimum number of stages. Another study performed heat integration of conventional hydrotreating and thermal indirect coupled column processes [85]. Like other literature, Carrasco-Suárez [83] found that the heat integration between two distillation columns, which were thermally coupled configurations of distillation columns, saved reboiler heat duty.

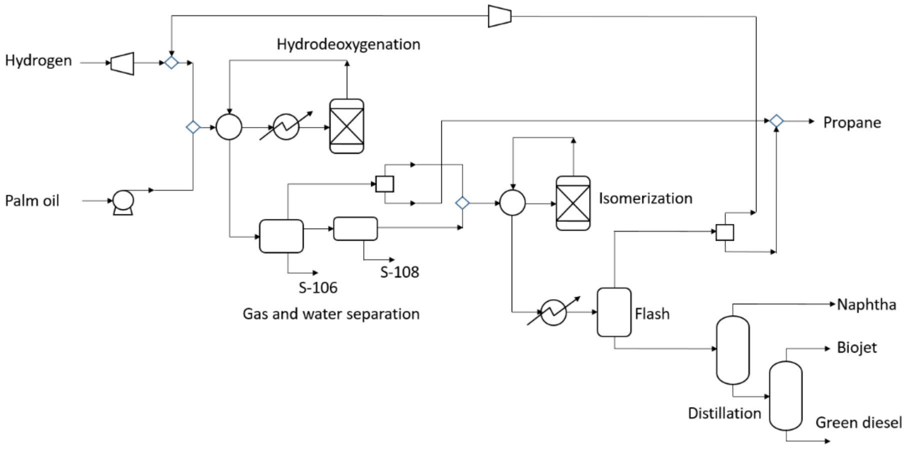

Figure 4: Bio-jet fuel production process by SuperPro Design [39].

Proposals for the co-processing of hydrotreating of vegetable oil and hydro desulphurization (HDS) of petroleum-based diesel have been put forth. These processes involve reactive distillation for the reaction and separation of light gases (i.e., H_2S and CO_2), followed by isomerization and hydrocracking to generate iso-paraffin and bio-jet fuel in the yield reactor [86].

Process intensification, achieved through reactive distillation, is explored for bio-jet production. In this scenario, long-chain hydrocarbons or BHD are subjected to cracking and isomerization within the reactive distillation while simultaneously separating light-chain hydrocarbons. This strategy aims to remove BHD from the light products, resulting in lower energy consumption [87]. The literature reviews related to such process simulation are shown in Table 4.

4.1.2 Process evaluation

Upon the comprehensive design of the bio-jet production process in various configurations, evaluations are conducted based on economic assessments. Key

Table 4: Process simulation of bio-jet production process

Raw Material	Model Compound	Reactor Model	Thermodynamic	Optimal Operating Conditions	Simulation Tools	Ref.
Castor oil	Palmitic acid, stearic acid, oleic acid, linoleic acid, linolenic acid, ricinoleic acid	Conversion reactor	Not mentioned	240 °C, 60 bar	Aspen Plus	[52]
Mixed vegetable oil (Camelina oil and Carinata oil)	Linolenic acid, oleic acid, linoleic acid	Conversion reactor	NTRL and Peng Robinson	400 °C, 92 bar	Aspen Plus	[77]
Waste cooking oil	Pentadecanoic acid, Nonadecanoic acid, Oleic Acid, Linoleic Acid	Conversion reactor	NTRL and Peng Robinson	400 °C, 92 bar	Aspen Plus	[78]
Microalgae oil	Oleic acid, linoleic acid, linolenic acid	Yield reactor	BK-10	410 °C, 50 bar	Aspen Plus	[79]
Palm oil	Tripalmitin, triolein, trilinolein, tristearin, trimyristin	Conversion reactor	Not mentioned	310 °C, 40 bar	SuperPro Designer	[81]
Soybean oil	Not mentioned	Yield reactor	Predictive Soave-Redlich-Kwong	300 °C, 30 bar	Aspen Plus	[82]
Waste cooking oil	Triglyceride, oleic acid, palmitic acid, linoleic acid	Yield reactor	Not mentioned	380 °C, 30 bar	Aspen Plus	[83]
Soybean oil	Not mentioned	Not mention	Not mentioned	240 °C, 60 bar	Aspen Plus	[84]
Jatropha curcas oil	Triolein, trilinolein, tripalmitin, tristearin	Yield reactor for hydrotreating, hydrocracking and isomerization	Not mentioned	320 °C, 80 bar for hydrotreating reactor, 480 °C, 80 bar for isomerization reactor	Aspen Plus	[85]
Vegetable oil	Triolein	Reactive distillation and Yield reactor	RK-ASPEN	350 °C, 30 bar	Aspen Plus	[86]
Jatropha curcas oil	Triolein, trilinolein, tripalmitin, tristearin	Yield reactor for hydrotreating, reactive distillation for hydrocracking and isomerization	Not mentioned	320 °C, 80 bar for hydrotreating reactor, 480 °C, 80 bar for isomerization	Aspen Plus	[87]
Rapeseed oil	Triolein	Yield reactor	Soave-Redlich-Kwong	350 °C, 40 bar	Aspen Plus	[88]

economic indicators, including total annual cost [77], [83], [86] total operating cost [88], [89] net present value (NPV), and minimum selling price [81], are scrutinized. The diversity of products generated in bio-jet production, such as naphtha, bio-jet, and diesel, necessitates a comparison between maximum diesel production and maximum bio-jet production across different feedstocks and plant capacity. Considering a cost breakdown, it is found that the equipment cost depends mainly on the hydrodeoxygenation section, which is approximately 49.19% [90]. The raw material cost substantially impacts overall operating costs [90]. In the case of maximum diesel production, the positive NPV and IRR were observed. On the contrary, a negative NPV was found with maximum bio-jet production [84]. In such a case, BHD production is preferable over bio-jet production [91]. An alternative approach involves a switch to waste cooking oil feedstocks, with considerations for cumulative cash flow and payback periods over ten years [78].

The minimum selling price of bio-jet fuel should be 1.37 $/L with an IRR of 10% when the plant capacity is low (45 thousand barrels/year). This price was still relatively high compared with petroleum-based jet fuel [81]. The results showed that the bio-jet production process could profit if the hydrogen's selling price was less than 2 $/kg, so the hydrogen price was a key factor [82]. It implies that raw material prices such as hydrogen [82] and vegetable oil [90]–[92] determine operating costs and profits. Li *et al.* [90] also found that the minimum selling price of bio-jet will drop by 41% when the camelina oil price decreases by 50%. The minimum selling price decreased from 0.5 $/L to 0.4 $/L with an increase in plant capacity of 100 to 300 million liters. However, a higher plant capacity of 400 million liters does not affect the minimum selling price. Discount rate also affects NPV when feedstock and plant capacity are constant. For example, NPV with Camelina oil price of 0.43 $/L, 225 million liters of plant capacity, and a 5% discount rate is $950,335. If the discount rate is 20%, the NPV is $328,197 [90]. Similarly, an NPV of 200 million dollars was obtained with a discount rate of 5%. NPV was decreased with an increase in the discount rate. In addition, NPV was zero, with a discount rate of 15% [78]. The literature reviews related to economic assessment are shown in Table 5.

Table 5: Economic assessment of the bio-jet production process

Raw Material	Price	Plant Capacity	Economic Indicator	Minimum Selling Price	Ref.
Waste cooking oil	Waste cooking oil price: 150$/tonne Hydrogen price: 1.6$/kg	1000 tonne/day of waste cooking oil	Rate of return: 15.91% Payback time: 5 years NPV: 6.4 million $/year with an interest rate of 8%	Bio-jet 0.71 $/L	[73]
Palm oil	Palm oil price: 0.289 – 0.405 $/kg Hydrogen price: 2 $/kg	75 thousand barrels/year	Rate of return: 10% Annual cost: 22.7 million $/year	Bio-jet 1.2 $/L	[75]
Soybean oil	Soybean oil price: 0.62 $/kg Hydrogen price: 2 $/kg	120 million liters/year	Payback time: 3.55 years	0.93 $/kg	[76]
Waste cooking oil	Hydrogen price: 1.8 $/kg	N.A.	Total annual cost: 7497523.1 $/year	N.A.	[77]
Camelina oil, Carinata oil, Jatropha oil	Camelina oil: 323 $/tonne Carinata oil: 356 $/tonne Jatropha oil: 254 $/tonne Hydrogen price: 1.21 $/kg	398 million liters/year maximum diesel production	Rate of return: 9.71%	Bio-jet: 0.4 $/L BHD: 0.98 $/L	[84]
Camelina oil	Camelina oil: 0.8 $/L Hydrogen price: 2.90 $/kg	252,000 tonne/year	NPV: 1047$ with a discount rate of 10% and bio-jet price of 0.6 $/L	Bio-jet: 1.06$/L	[85]
Jatropha oil	Jatropha oil price: 650 Euro/tonne	0.5 million ton/year of vegetable oil	Tonetal production cost: 1725 Euro/tonne of bio-jet	Bio-jet: 735 €/tonne	[86]
Jatropha oil	Jatropha oil price: 2.06 $/gal	Bio-jet 44 million gal/year	Total capital investment: 341 million $	Bio-jet: 1.00 $/L	[87]

5 Future Simulation Needs

Machine learning (ML) is another simulation area that gives some advantages to reducing experimental time by avoiding the trial and error method, which is time-consuming. Unlike traditional methods, such as response surface methodology (RSM), ML can be learned from previous studies to identify patterns or predict process performance on unseen datasets. ML can be effectively applied in many fields, including chemistry and chemical engineering. For example, supervised ML emerges as a potent tool for predicting chemical properties from Simplified Molecular-Input Line-Entry System (SMILES) strings [93], exemplifying its broad applicability. Regression analyses within ML frameworks offer predictive insights into process performance concerning yield and purity, linked to operating parameters.

Artificial neural networks (ANNs) represent a robust ML algorithm, capable of modeling after training on data. The structure of ANNs, featuring input data, multi-layers, and output data interconnected by weight matrices and bias vectors, facilitates predictive modeling. For bio-jet production, ANNs have been applied to forecast bio-jet yield based on input parameters such as the molar ratio of ethanol to oil, reaction time, and microwave power. All data were divided into training, validation, and testing. The ANN structure with three hidden layers was proposed based on the minimum mean square error and the highest coefficient correlation (R square). Comparative analyses highlight the superiority of ANNs over response surface methodology (RSM) in terms of model fit and prediction accuracy [94].

Convolutional neural networks (CNNs), another variant of neural networks, consist of convolutional, pooling, and connected layers. It can reduce overfitting compared with ANN. CNN is widely used for image classification. However, it can be applied to predict the hydrocracking process for bio-jet production. Input parameters were 74 types of raw materials, hydrogen flow rate, and operating conditions of reactors and distillation columns. The output parameters were production yield (i.e., light hydrocarbon, light naphtha, heavy naphtha, kerosene, and diesel) and outlet temperature. The data was preprocessed by eliminating the missing data. The results demonstrate the adeptness of CNNs in providing an excellent fit to time series data collected over specific durations, from December 2017 until March 2019, in terms of mean absolute error (MAE) [95].

The synthesis of empirical models for predicting molecular structure and functional group properties via ML methodologies addresses the limitations of traditional analytical instruments. Gas chromatography, Raman spectroscopy, and FTIR are pivotal for testing new components. Yet, ML offers a viable solution by training on composition datasets and properties (i.e., H/C ratio, molecular weight, flash point, freezing point, and cetane number). The Python package Scikit-Learn was used to train and test the dataset. Algorithms such as Random Forest, Adaptive Boosting, and Regression were studied. The best model can predict the properties in terms of the lowest root mean square error and mean absolute error [96].

The novel application of ML extends to predicting the properties of new chemicals through learning known molecular structures. The atom features such as atom type, hybridization, and number of bonds can be classified as nodes in molecular graphs. Then, graph neural networks (GNN) using RDKit in Python can be used to predict properties such as boiling points [97].

Notwithstanding these advancements, the divergence between process simulation and ML lies in data requirements. The process simulation requires the mathematical model of unit operations, model parameters, thermodynamic model, kinetic data, and process conditions. Physical, chemical, and biological knowledge should be understood deeply so the simulation computes correctly. However, a large dataset is required to develop a model for training, testing, and validation datasets in the case of ML. If the inputs are known, the output can be predicted. Thus, integrating data science with chemical engineering becomes imperative to forecast production yield and properties, particularly in scenarios where novel chemicals or materials are discovered. The knowledge of this area for bio-jet fuel production and fuel properties is still challenging.

6 Conclusions

This review provides valuable insights into the production of bio-jet fuel from vegetable oils. An overview of diverse feedstocks for bio-jet fuel production has been presented. The updated and detailed information on ASTM-certified production pathways has been elucidated. Notably, the HEFA feedstock stands out as the predominant and commercially produced bio-jet fuel via the oil-to-jet process. The HEFA process entails the conversion of triglycerides in vegetable oils into bio-jet fuel through hydroprocessing reactions, encompassing hydrodeoxygenation, decarboxylation, and decarbonylation. Subsequent stages involve the cracking and isomerization of hydroprocessed hydrocarbons, yielding bio-jet fuel products suitable for blending with petroleum-based jet fuel.

The exploration of modeling and simulation in bio-jet fuel production from vegetable oils has been undertaken. Computational Fluid Dynamics (CFD) modeling of hydroprocessing reactors is frequently employed to assess reactor performance and refine design. The optimization of reactors involves meticulous consideration of various process parameters, with a particular focus on the concentration and temperature profiles of chemicals. Despite its utility, CFD modeling faces limitations due to the absence of kinetic rate data, necessitating actual experimental tests. Future research should emphasize considerations of hydrodynamic effects, kinetic rate data, and mass transfer to comprehensively understand transport phenomena.

In contrast to CFD modeling, process simulation using software like Aspen Plus concentrates on the holistic design of the bio-jet fuel production process. Operating conditions for hydroprocessing reactors are typically derived from experimental data and literature sources. Consequently, the prediction of maximum yield relies on available process conditions. A sensitivity analysis is often required for a process that generates multiple products alongside bio-jet fuel as it helps gauge the economic implications of varying process conditions. Notably, the challenges associated with Aspen Plus design persist due to incomplete or missing data on vegetable oils. Thermodynamic models play a vital role in ensuring accurate predictions of the chemical and physical properties of involved compounds. The future of process simulation points towards the integration of Machine Learning (ML). With its potential to diminish the need for extensive experimental sets, ML emerges as a promising avenue for predicting yields and missing properties. This transition to ML is contingent on high-quality datasets and effective training, offering a more efficient and predictive approach to bio-jet fuel production processes.

Acknowledgments

This work was funded by King Mongkut's University of Technology North Bangkok, Contract no. KMUTNB-67-BASIC-19.

Author Contributions

L.S.: methodology, writing – original draft; SS.: conceptualization, methodology, writing – original draft, writing – reviewing and editing; K.T.: supervision; S.A.: supervision; All authors have read and agreed to the published version of the manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

References

[1] A United Nations Specialized Agency, "Air traffic recovery is fast – approaching pre-pandemic level," 2021. [Online]. Available: https://www.icao.int/Newsroom/Pages/Air-traffic-recovery-is-fastapproaching-prepandemic-levels.aspx

[2] U.S. Department of Energy, "Sustainable aviation fuel: Review of technical pathways report," 2020. [Online]. Available: https://www.energy.gov/sites/default/files/2020/09/f78/beto-sust-aviation-fuel-sep-2020.pdf

[3] A. W. Schäfer, A. D. Evans, T. G. Reynolds, and L. Dray, "Costs of mitigating CO_2 emissions from passenger aircraft," *Nature Climate Change*, vol. 6, no. 4, pp. 412–417, 2016, doi: 10.1038/nclimate2865.

[4] J. I. Hileman, D. S. Ortiz, J. T. Bartis, H. M. Wong, P. E. Donohoo, M. A. Weiss, and I. A. Waitz, "Near-Term Feasibility of Alternative Jet Fuels," 2009. [Online]. Available: https://www.rand.org/pubs/technical_reports/TR554.html

[5] J. Yang, Z. Xin, Q. (Sophia) He, K. Corscadden, and H. Niu, "An overview on performance characteristics of bio-jet fuels," *Fuel*, vol. 237, pp. 916–936, Feb. 2019, doi: 10.1016/j.fuel.2018.10.079.

[6] T. Nunlist, “Flying High: China’s Aviation Industry is Becoming a Global Force,” 2024. [Online]. Available: https://english.ckgsb.edu.cn/knowledge/article/flying-high-chinas-aviation-industry-is-becoming-a-global-force/

[7] R. Jiménez, “RefuelEU aviation initiative: Council adopts new law to decarbonise the aviation sector – Consilium,” 2024. [Online]. Available: https://www.consilium.europa.eu/en/press/press-releases/2023/10/09/refueleu-aviation-initiative-council-adopts-new-law-to-decarbonise-the-aviation-sector/

[8] D. S. Lee, D. W. Fahey, P. M. Forster, P. J. Newton, R. C. N. Wit, L. L. Lim, B. Owen, and R. Sausen, “Aviation and global climate change in the 21st century,” *Atmospheric Environment*, vol. 43, no. 22–23, pp. 3520–3537, Jul. 2009, doi: 10.1016/j.atmosenv.2009.04.024.

[9] U.S. Energy Information Administration, “Monthly Energy Review 2017,” 2017. [Online]. Available: http://www.eia.gov/totalenergy/data/monthly/#consumption.

[10] J. I. Hileman and R. W. Stratton, “Alternative jet fuel feasibility,” *Transport Policy*, vol. 34, pp. 52–62, Jul. 2014, doi: 10.1016/j.tranpol.2014.02.018.

[11] K. Atsonios, M. A. Kougioumtzis, K. D. Panopoulos, and E. Kakaras, “Alternative thermochemical routes for aviation biofuels via alcohols synthesis: Process modeling, techno-economic assessment and comparison,” *Applied Energy*, vol. 138, pp. 346–366, Jan. 2015, doi: 10.1016/j.apenergy.2014.10.056.

[12] I. H. Choi, K. R. Hwang, J. S. Han, K. H. Lee, J. S. Yun, and J. S. Lee, “The direct production of jet-fuel from non-edible oil in a single-step process,” *Fuel*, vol. 158, pp. 98–104, Oct. 2015, doi: 10.1016/j.fuel.2015.05.020.

[13] ASTM International, “ASTM D975-12a standard specification for diesel fuel oils,” 2013. [Online]. Available: https://www.astm.org/d0975-23a.html

[14] U.S. Department of Defense, “Detail specification: turbine fuel, aviation, kerosene type, JP-8 (NATO F-34), NATO F-35, and JP-8þ100 (NATO F-37),” 2011. [Online]. Available: https://publishers.standardstech.com/stgnet

[15] L. H. Duong, I. K. Reksowardojo, T. H. Soerawidjaja, O. Fujita, G. F. Neonufa, T. T.G. Nguyen, and T. Prakoso, “Soap-derived biokerosene as an aviation alternative fuel: Production, composition, and properties of various blends with jet fuel,” *Chemical Engineering and Processing - Process Intensification*, vol. 153, Jul. 2020, Art. no. 107980, doi: 10.1016/j.cep.2020.107980.

[16] C. H. Lin, Y. K. Chen, and W. C. Wang, “The production of bio-jet fuel from palm oil derived alkanes,” *Fuel*, vol. 260, Jan. 2020, Art. no. 116345, doi: 10.1016/j.fuel.2019.116345.

[17] H. Liu, C. Zhang, H. Tian, L. Li, X. Wang, and T. Qiu, “Environmental and techno-economic analyses of bio-jet fuel produced from jatropha and castor oilseeds in China,” *International Journal of Life Cycle Assessment*, vol. 26, pp. 1071–1084, 2021, doi: 10.1007/s11367-021-01914-0.

[18] N. Vela-García, D. Bolonio, M. J. García-Martínez, M. F. Ortega, D. A. Streitwieser, and L. Canoira, “Biojet fuel production from oleaginous crop residues: Thermoeconomic, life cycle and flight performance analysis,” *Energy Conversion and Management*, vol. 244, 2021, Art. no. 114534, doi: 10.1016/j.enconman.2021.114534.

[19] U. Wangrakdiskul and N. Yodpijit, “Trends analysis and future of sustainable palm oil in Thailand,” *Applied Science and Engineering Congress*, Vol.8, No.1, pp. 21-32, 2015.

[20] P. Muanruksa, J. Winterburn, and P. Kaewkannetra, “Biojet fuel production from waste of palm oil mill effluent through enzymatic hydrolysis and decarboxylation,” *Catalysts*, vol. 11, no. 1, 2021, Art. no. 78, doi: 10.3390/catal11010078.

[21] N. Sarkar, S. K. Ghosh, S. Bannerjee, and K. Aikat, “Bioethanol production from agricultural wastes: An overview,” *Renewable Energy*, vol. 37, no. 1, pp. 19–27, Jan. 2012, doi: 10.1016/j.renene.2011.06.045.

[22] A. Gupta and J. P. Verma, “Sustainable bio-ethanol production from agro-residues: A review,” *Renewable and Sustainable Energy Reviews*, vol. 41, pp. 550–567, Jan. 2015, doi: 10.1016/j.rser.2014.08.032.

[23] T. L. T. Nguyen, J. E. Hermansen, and L. Mogensen, “Environmental performance of crop residues as an energy source for electricity production: The case of wheat straw in Denmark,” *Applied Energy*, vol. 104, pp. 663–641, 2013, doi: 10.1016/j.apenergy.2012.11.057.

[24] C. S. K. Lin, L. A. Pfaltzgraff, L. Herrero-Davila, E. B. Mubofu, S. Abderrahim, J. H. Clark, A. A. Koutinas, N. Kopsahelis, K. Stamatelatou, F. Dickson, S. Thankappan, Z. Mohamed, R. Brocklesby, and R. Luque, "Food waste as a valuable resource for the production of chemicals, materials and fuels. Current situation and global perspective," *Energy and Environmental Science*, vol. 6, no. 2, pp. 426–464, 2013, doi: 10.1039/c2ee23440h.

[25] B. K. Adhikari, S. Barrington, and J. Martinez, "Predicted growth of world urban food waste and methane production," *Waste Management and Research*, vol. 24, no. 5, pp. 421–433, 2006, doi: 10.1177/0734242X06067767.

[26] S. Kirdponpattara, S. Chuetor, M. Sriariyanun, and M. Phisalaphong, "Bioethanol production by Pichia stipitis Immobilized on water hyacinth and thin-shell silk cocoon," *Applied Science and Engineering Progress*, vol. 15, no. 3, 2022, Art. no. 4662.

[27] S. R. Couto and M. Á. Sanromán, "Application of solid-state fermentation to food industry-A review," *Journal of Food Engineering*, vol. 76, no. 3, pp. 291–302, 2006, doi: 10.1016/j.jfoodeng.2005.05.022.

[28] L. A. Sargeant, M. Mardell, K. M. Saad-Allah, A. H. Hussein, F. Whiffin, F. Santomauro, and C. J. Chuck, "Production of lipid from depolymerised lignocellulose using the biocontrol yeast, rhodotorula minuta: The fatty acid profile remains stable irrespective of environmental conditions," *European Journal of Lipid Science and Technology*, vol. 118, no. 5, pp. 777–787, 2016, doi: 10.1002/ejlt.201500143.

[29] D. P. Ho, H. H. Ngo, and W. Guo, "A mini review on renewable sources for biofuel," *Bioresource Technology*, vol. 169, pp. 742–749, 2014, doi:10.1016/j.biortech.2014.07.022.

[30] I. Lewandowski, J. M. O. Scurlock, E. Lindvall, and M. Christou, "The development and current status of perennial rhizomatous grasses as energy crops in the US and Europe," *Biomass Bioenergy*, vol. 25, no. 4, pp. 335–361, 2003, doi: 10.1016/S0961-9534(03)00030-8.

[31] C. Sorensen, "Petroleum-Based Jet Fuel Production & SAF" 2024. [Online]. Available: https://lee-enterprises.com/petroleum-based-jet-fuel-production-saf/

[32] K. J. Vicari, S. S. Tallam, T. Shatova, K. K. Joo, C. J. Scarlata, D. Humbird, E. J. Wolfrum, and G. T. Beckham, "Uncertainty in techno-economic estimates of cellulosic ethanol production due to experimental measurement uncertainty," *Biotechnol Biofuels*, vol. 5, 2012, Art. no. 23, doi: 10.1186/1754-6834-5-23.

[33] M. Y. Koh and T. I. Tinia, "A review of biodiesel production from *Jatropha curcas* L. oil," *Renewable and Sustainable Energy Reviews*, vol. 15, no. 5, pp. 2240–2251, 2011, doi: 10.1016/j.rser.2011.02.013.

[34] D. R. Shonnard, L. Williams, and T. N. Kalnes, "Camelina-derived jet fuel and diesel: Sustainable advanced biofuels," *Environmental Progress &Sustainable Energy*, vol. 29, no. 3, pp. 382–392, 2010, doi: 10.1002/ep.10461.

[35] Z. Yaakob, M. Mohammad, M. Alherbawi, Z. Alam, and K. Sopian, "Overview of the production of biodiesel from Waste cooking oil," *Renewable and Sustainable Energy Reviews*, vol. 18. pp. 184–193, 2013, doi: 10.1016/j.rser.2012.10.016.

[36] M. G. Kulkarni and A. K. Dalai, "Waste cooking oil - An economical source for biodiesel: A review," *Industrial and Engineering Chemistry Research*, vol. 45, no. 9. pp. 2901–2913, 2006, doi: 10.1021/ie0510526.

[37] L. Brennan and P. Owende, "Biofuels from microalgae-A review of technologies for production, processing, and extractions of biofuels and co-products," *Renewable and Sustainable Energy Reviews*, vol. 14, no. 2, pp. 557–577, 2010, doi: 10.1016/j.rser.2009.10.009.

[38] L. A. Ribeiro and P. P. Da Silva, "Surveying techno-economic indicators of microalgae biofuel technologies," *Renewable and Sustainable Energy Reviews*, vol. 25, pp. 89–96, 2013. doi: 10.1016/j.rser.2013.03.032.

[39] C. J. Chuck, J. L. Wagner, and R. W. Jenkins, "Biofuels from Microalgae," in *Chemical Processes for a Sustainable Future*, T. Letcher, J. Scott, and D. Patterson, Eds. The Royal Society of Chemistry, London, UK, pp. 425–442, 2014, doi: 10.1039/BK9781849739757-00423.

[40] T. Wuttilerts, S. Chulalaksananukul, P. Peerapongpipat, and P. Suksommanat, "Evaluation of biodiesel production using oil feedstock from contaminated

macro algae in shrimp farming," *Applied Science and Engineering Progress*, vol. 12, no. 3, pp. 179–185, 2019, doi: 10.14416/j.ijast.2018.11.005.

[41] R. Davis, A. Aden, and P. T. Pienkos, "Techno-economic analysis of autotrophic microalgae for fuel production," *Applied Energy*, vol. 88, no. 10, pp. 3524–3531, 2011. doi: 10.1016/j.apenergy.2011.04.018.

[42] H. Wei, W. Liu, X. Chen, Q. Yang, J. Li, and H. Chen, "Renewable bio-jet fuel production for aviation: A review," *Fuel*, vol. 254. 2019, Art. no. 115599, doi: 10.1016/j.fuel.2019.06.007.

[43] ICAO, "Conversion processes," 2024. [Online]. Available: https://www.icao.int/environmental-protection/GFAAF/Pages/Conversion-processes.aspx

[44] K. R. Weiss, "Advancing 'Alcohol To Jet' To Full Replacement Fuel (ATJ-SKA)," 2020. [Online]. Available: https://www.icao.int/Meetings/Stocktaking2020/Documents/ICAO Stocktaking %202020 - 3.3.7 - Kevin Weiss.pdf

[45] Swedish Biofuels AB, "Swedish Biofuels AB," 2024. [Online]. Available: https://swedishbiofuels.se/projects/biological-fully-synthetic-jet

[46] CAAFI, "Fuel Qualification," 2024. [Online]. Available: https://www.caafi.org/focus_areas/fuel_qualification.html

[47] A. de Klerk "Aviation turbine fuels through the fischertropsch process," in *Biofuels for Aviation Feedstocks, Technology and Implementation*. Massachusetts: Academic Press, pp. 241–259, 2016.

[48] P. Maki-Arvela, M. Martinez-Klimov, D. Murzin, "Hydroconversion of fatty acids and vegetable ois for production of jet fuels," *Fuel*, vol. 306, 2021, Art. no. 121673.

[49] K. Ng, D. Faroog, A. Yang, "Global biorenewable development strategies for sustainable aviation fuel production" *Renewable and Sustainable Energy Reviews*, vol. 105, 2021, Art. no. 111502.

[50] P. R. Robinson and G. E. Dolbear, "Hydrotreating and hydrocracking: Fundamentals" in *Practice Advance in Petroleum Processing.* New York: Springer, pp. 177–218, 2006, doi: 10.1007/978-0-387-25789-1_7.

[51] H. Kittel, J. Horský, and P. Šimáček, "Properties of selected alternative petroleum fractions and sustainable aviation fuels" *Process*, vol. 11, 2023, Art. no. 935, doi: 10.3390/pr11030935.

[52] C. Gutiérrez-Antonio, F. Israel Gómez-Castro, J. G. Segovia-Hernández, and A. Briones-Ramírez, "Simulation and optimization of a biojet fuel production process," *Computer Aided Chemical Engineering*, vol. 32, pp. 13–18, 2013, doi: 10.1016/B978-0-444-63234-0.50003-8.

[53] Ł. Jęczmionek and K. Porzycka-Semczuk, "Hydrodeoxygenation, decarboxylation and decarbonylation reactions while co-processing vegetable oils over a NiMo hydrotreatment catalyst. Part I: Thermal effects - Theoretical considerations," *Fuel*, vol. 131, pp. 1–5, 2014, doi: 10.1016/j.fuel.2014.04.055.

[54] A. Galadima and O. Muraza, "Catalytic upgrading of vegetable oils into jet fuels range hydrocarbons using heterogeneous catalysts: A review," *Journal of Industrial and Engineering Chemistry*, vol. 29, pp. 12–23, 2015, doi: 10.1016/j.jiec.2015.03.030.

[55] V. Itthibenchapong, A. Srifa, R. Kaewmeesri, P. Kidkhunthod, and K. Faungnawakij, "Deoxygenation of palm kernel oil to jet fuel-like hydrocarbons using Ni-MoS_2/γ-Al_2O_3 catalysts," *Energy Conversion and Management*, vol. 134, pp. 188–196, 2017, doi: 10.1016/j.enconman.2016.12.034.

[56] A. Sonthalia and N. Kumar, "Hydroprocessed vegetable oil as a fuel for transportation sector: A review," *Journal of the Energy Institute*, vol. 92, no. 1, pp. 1–17, 2019, doi: 10.1016/j.joei.2017.10.008.

[57] I-H. Choi, J-S Lee, C-U. Kim, T-W. Kim, K-Y Lee, and K-R. Hwang, "Production of bio-jet fuel range alkanes from catalytic deoxygenation of Jatropha fatty acids on a WOx/Pt/TiO_2 catalyst," *Fuel*, vol. 215, pp. 675–685, 2018, doi: 10.1016/j.fuel.2017.11.094.

[58] M. Alherbawi, G. McKay, H. R. Mackey, and T. Al-Ansari, "Jatropha curcas for jet biofuel production: Current status and future prospects," *Renewable and Sustainable Energy Reviews*, vol. 135, 2021, Art. no. 110396. doi: 10.1016/j.rser.2020.110396.

[59] M. C. Vásquez, E. E. Silva, and E. F. Castillo, "Hydrotreatment of vegetable oils: A review of the technologies and its developments for jet biofuel production," *Biomass and Bioenergy*,

vol. 105, pp. 197–206, 2017, doi: 10.1016/j.biombioe.2017.07.008.

[60] T. Morgan, D. Grubb, E. Santillan-Jimenez, and M. Crocker, "Conversion of triglycerides to hydrocarbons over supported metal catalysts," *Topic in Catalysis*, vol. 53, no. 11–12, pp. 820–829, 2010, doi: 10.1007/s11244-010-9456-1.

[61] Zhang Ze, Cheng J, Zhu Y, Guo H, and Yang W. "Jet fuel range hydrocarbons production through competitive pathways of hydrocracking and isomerization over HPW-Ni/MCM-41 catalyst," *Fuel*, vol.269, 2020, Art. no. 117465, doi: 10.1016/j.fuel.2020.117465.

[62] S. Khan, A. N. Kay Lup, K. M. Qureshi, F. Abnisa, W. M. A. Wan Daud, and M. F. A. Patah, "A review on deoxygenation of triglycerides for jet fuel range hydrocarbons," *Journal of Analytical and Applied Pyrolysis*, vol. 140, pp. 1–24, 2019, doi: 10.1016/j.jaap.2019.03.005.

[63] C. A. Scaldaferri and V. M. D. Pasa, "Hydrogen-free process to convert lipids into bio-jet fuel and green diesel over niobium phosphate catalyst in one-step," *Chemical Engineering Journal*, vol. 370, pp. 98–109, 2019, doi: 10.1016/j.cej.2019.03.063.

[64] L. M. de Souza, P. A. S. Mendes, and D. A. G. Aranda, "Oleaginous feedstocks for hydro-processed esters and fatty acids (HEFA) biojet production in southeastern Brazil: A multi-criteria decision analysis," *Renewable Energy*, vol. 149, pp. 1339–1351, 2020, doi: 10.1016/j.renene.2019.10.125.

[65] C. J. Chuck, *Biofuels for Aviation Feedstocks, Technology and Implementation*. Massachusetts: Academic Press, vol. 1, pp. 855–856, 2016.

[66] C. Gutiérrez-Antonio, F. I. Gómez-Castro, A. G. Romero-Izquierdo, and S. Hernández, "Energy integration of a hydrotreating process for the production of biojet fuel," *Computer Aided Chemical Engineering*, vol. 38, pp. 127–132, 2016, doi: 10.1016/B978-0-444-63428-3.50026-6.

[67] M. Makcharoen, A. Kaewchada, N. Akkarawatkhoosith, and A. Jaree, "Biojet fuel production via deoxygenation of crude palm kernel oil using Pt/C as catalyst in a continuous fixed bed reactor," *Energy Conversion and Management: X*, vol. 12, 2021, Art. no. 100125, doi: 10.1016/j.ecmx.2021.100125.

[68] D. Chehadeh, X. Ma, and H. Al Bazzaz, "Recent progress in hydrotreating kinetics and modeling of heavy oil and residue: A review," *Fuel*, vol. 334, 2023, Art. no. 126404, doi: 10.1016/j.fuel.2022.126404.

[69] L. Attanatho, "Performances and kinetic studies of hydrotreating of bio-oils in microreactor," 2012. [Online]. Available: https://ir.library.oregonstate.edu/concern/graduate_thesis_or_dissertations/gx41mp382?locale=en

[70] Y. Muharam, O. A. Nugraha, and D. Leonardi, "Modelling of a hydrotreating reactor to produce renewable diesel from non-edible vegetable oils," *Chemical Engineering Transaction*, vol. 56, pp. 1561–1566, 2017, doi: 10.3303/CET1756261.

[71] A. R. K. Gollakota, M. D. Subramanyam, N. Kishore, and S. Gu, "CFD simulations on the effect of catalysts on the hydrodeoxygenation of bio-oil," *RSC Advances*, vol. 5, no. 52, pp. 41855–41866, 2015, doi: 10.1039/c5ra02626a.

[72] M. D. Subramanyam, A. R. K. Gollakota, and N. Kishore, "CFD simulations of catalytic hydrodeoxygenation of bio-oil using Pt/Al_2O_3 in a fixed bed reactor," *RSC Advances*, vol. 5, no. 110, pp. 90354–90366, 2015, doi: 10.1039/c5ra14985a.

[73] A. Tirado, F. Trejo, and J. Ancheyta, "Simulation of bench-scale hydrotreating of vegetable oil reactor under non-isothermal conditions," *Fuel*, vol. 275, 2020, Art. no. 117960, doi: 10.1016/j.fuel.2020.117960.

[74] Y. Muharam and R. T. Adevia, "Modelling and simulation of a slurry bubble column reactor for green fuel production via hydrocracking of vegetable oil," in *E3S Web of Conferences*, 2018, Art. no. 02032, doi: 10.1051/e3sconf/20186702032.

[75] E. Quiroz-Pérez, C. Gutiérrez-Antonio, J. A. de Lira-Flores, and R. Vázquez-Román, "A thermal-hydrodynamic model to evaluate the potential of different tray designs for production of renewable aviation fuel through reactive distillation," *Chemical Engineering and Processing - Process Intensification*, vol. 166, 2021, Art. no. 108482, doi: 10.1016/j.cep.2021.108482.

[76] N. Phichitsurathaworn, L. Simasatitkul, S. Amornraksa, A. Anantpinijwatna, P. Charoensuppanimit, and S. Assabumrungrat, "Techno-economic analysis of co-production of bio-hydrogenated diesel from

palm oil and methanol," *Energy Conversion and Management*, vol. 244, 2021, Art. no. 114464, doi: 10.1016/j.enconman.2021.114464.

[77] P. L. Chu, C. Vanderghem, H. L. MacLean, and B. A. Saville, "Process modeling of hydrodeoxygenation to produce renewable jet fuel and other hydrocarbon fuels," *Fuel*, vol. 196, pp. 298–305, 2017, doi: 10.1016/j.fuel.2017.01.097.

[78] E. Barbera, R. Naurzaliyev, A. Asiedu, A. Bertucco, E. P. Resurreccion, and S. Kumar, "Techno-economic analysis and life-cycle assessment of jet fuels production from waste cooking oil via in situ catalytic transfer hydrogenation," *Renewable Energy*, vol. 160, pp. 428–449, 2020, doi: 10.1016/j.renene.2020.06.077.

[79] A. Gómez-De la Cruz, A. G. Romero-Izquierdo, C. Gutiérrez-Antonio, F. I. Gómez-Castro, and S. Hernández, "Modelling of the hydrotreating process to produce renewable aviation fuel from micro-algae oil," *Computer Aided Chemical Engineering*, vol. 40, pp. 655–660, 2017, doi: 10.1016/B978-0-444-63965-3.50111-2.

[80] UOP, "UOP Ecofining™ process for sustainable aviation fuel," USA, 2021. [Online]. Available: https://uop.honeywell.com/

[81] E. Martinez-Hernandez, L. F. Ramírez-Verduzco, M. A. Amezcua-Allieri, and J. Aburto, "Process simulation and techno-economic analysis of bio-jet fuel and green diesel production — Minimum selling prices," *Chemical Engineering Research and Design*, vol. 146, pp. 60–70, 2019, doi: 10.1016/j.cherd.2019.03.042.

[82] I. Z. Ambrosio, B. R. Margarida, and L. F. L. Luz, "Simulation and optimization ff biojet fuel production through single-step route and residual raw material," *Chemical Enginering Transaction*, vol. 99, pp. 613–618, 2023, doi: 10.3303/CET2399103.

[83] M. T. Carrasco-Suárez, A. G. Romero-Izquierdo, C. Gutiérrez-Antonio, F. I. Gómez-Castro, and S. Hernández, "Production of renewable aviation fuel by waste cooking oil processing in a biorefinery scheme: Intensification of the purification zone," *Chemical Engineering and Processing - Process Intensification*, vol. 181, 2022, Art. no. 109103, doi: 10.1016/j.cep.2022.109103.

[84] C. Gutiérrez-Antonio, F. I. Gómez-Castro, S. Hernández, and A. Briones-Ramírez, "Intensification of a hydrotreating process to produce biojet fuel using thermally coupled distillation," *Chemical Engineering and Processing: Process Intensification*, vol. 88, pp. 29–36, 2015, doi: 10.1016/j.cep.2014.12.002.

[85] M. García-Sánchez, M. Sales-Cruz, T. Lopez-Arenas, T. Viveros-García, and E. S. Pérez-Cisneros, "An intensified reactive separation process for bio-jet diesel production," *Processes*, vol. 7, no. 10, 2019, Art. no. 655, doi: 10.3390/pr7100655.

[86] C. Gutiérrez-Antonio, A. G. Romero-Izquierdo, F. I. Gómez-Castro, S. Hernández, and A. Briones-Ramírez, "Simultaneous energy integration and intensification of the hydrotreating process to produce biojet fuel from jatropha curcas," *Chemical Engineering and Processing: Process Intensification*, vol. 110, pp. 134–145, 2016, doi: 10.1016/j.cep.2016.10.007.

[87] C. Gutiérrez-Antonio, M. L. Soria Ornelas, F. I. Gómez-Castro, and S. Hernández, "Intensification of the hydrotreating process to produce renewable aviation fuel through reactive distillation," *Chemical Engineering and Processing: Process Intensification*, vol. 124, pp. 122–130, 2018, doi: 10.1016/j.cep.2017.12.009.

[88] Z. Béalu, "Process simulation and optimization of alternative liquid fuels production: A techno-economic assessment of the production of HEFA Jet Fuel," M.S. Thesis, University of Kaiserslautern, Germany, 2017.

[89] A. P. M. M. Diniz, R. Sargeant, and G. J. Millar, "Stochastic techno-economic analysis of the production of aviation biofuel from oilseeds," *Biotechnology for Biofuels*, vol. 11, no. 1, 2018, Art. no. 161, doi: 10.1186/s13068-018-1158-0.

[90] X. Li, E. Mupondwa, and L. Tabil, "Technoeconomic analysis of biojet fuel production from camelina at commercial scale: Case of Canadian Prairies," *Bioresource Technology*, vol. 249, pp. 196–205, 2018, doi: 10.1016/j.biortech.2017.09.183.

[91] K. M. Zech, S. Dietrich, M. Reichmuth, W. Weindorf, and F. Müller-Langer, "Techno-economic assessment of a renewable bio-jet-fuel production using power-to-gas," *Applied Energy*, vol. 231, pp. 997–1006, 2018, doi: 10.1016/

j.apenergy.2018.09.169.

[92] L. Tao, A. Milbrandt, Y. Zhang, and W. C. Wang, "Techno-economic and resource analysis of hydroprocessed renewable jet fuel," *Biotechnolology for Biofuels*, vol. 10, no. 1, 2017, Art. no. 261, doi: 10.1186/s13068-017-0945-3.

[93] Z. Li, M. Jiang, S. Wang, and S. Zhang, "Deep learning methods for molecular representation and property prediction," *Drug Discovery Today*, vol. 27, no. 12, 2022, Art. no. 103373, doi: 10.1016/j.drudis.2022.103373.

[94] M. Y. Ong, S. Nomanbhay, F. Kusumo, R. M. H. Raja Shahruzzaman, and A. H. Shamsuddin, "Modeling and optimization of microwave-based bio-jet fuel from coconut oil: Investigation of response surface methodology (RSM) and artificial neural network methodology (ANN)," *Energies,* vol. 14, no. 2, 2021, Art. no. 295, doi: 10.3390/en14020295.

[95] W. Song, V. Mahalec, J. Long, M. Yang, and F. Qian, "Modeling the hydrocracking process with deep neural networks," *Industrial & Engineering Chemistry Research*, vol. 59, no. 7, pp. 3077–3090, 2020, doi: 10.1021/acs.iecr.9b06295.

[96] M. Mayer, "Predicting properties of bio-jet fuels using machine learning and ATR-FTIR spectroscopy," M.S. Thesis, Oregon State University, USA, 2021.

[97] J. G. Rittig, Q. Gao, M. Dahmen, A. Mitsos, and A. M. Schweidtmann, "Graph neural networks for the prediction of molecular structure-property relationships," 2023. [Online]. Available: http://arxiv.org/abs/2208.04852