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Review

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Recent Advances in Combustion Chemistry of Biofuels: A Review

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Abstract: Renewable energy sources such as biofuels play a critical role in climate change mitigation and in meeting the rising global energy demand. To achieve carbon neutrality, biofuels such as bioethanol, biodiesel and biogas are a promising solution because they are renewable. The use of biofuels has potential to significantly reduce reliance on fossil fuels and contribute to increased access to clean and affordable energy as envisioned in sustainable development goal 7 (SDG 7). However, their effective utilization is constrained by challenges in combustion kinetics, fuel property variability, and emission trade-offs arising from complex reaction pathways compared to conventional fuels. The present study provides a concise review of key aspects in combustion kinetics and mechanisms of bioethanol, biodiesel and biogas. Comparative analysis is provided to highlight inconsistencies in reported findings and limitations in current methodologies. The study proposes ways to address these challenges through combining fundamental research, computational modelling and experimental innovation to accelerate the transition toward a cleaner energy future.

Keywords: biodiesel; bioethanol; biogas; combustion; kinetics; computational modeling

1. Introduction

1.1. Background on Biofuels

Energy is a key enabler of development, however reliance on fossil fuels globally is detrimental to the environment and accelerates climate change [1]. This has necessitated a global energy transition involves a shift from fossil fuels to renewable energy sources. This shift is motivated by the need for sustainable development, volatility in the supply of fossil fuel and concerns about fossil energy reserve depletion [2]. The main objectives of this transition is to reduce greenhouse gas emissions that contribute to climate change and global warming [3] as well as safeguard energy security by reducing reliance on finite fossil energy sources [4]. Biomass, an abundant resource, has emerged as one of the most promising renewable energy source capable of contributing to this global energy transition [5]. This versatile resource can be converted into a variety of biofuels through different direct combustion, thermochemical, biochemical, and chemical conversion processes. Biofuels, are considered a clean energy resource, derived from organic matter, agricultural waste, plants and algae. They present a significant opportunity for the mitigation of problems associated with the utilization of fossil fuels. Biofuels emit less greenhouse gases (GHG) and are in general more eco-friendly (non-toxic, sulfur-free, biodegradable) than their fossil fuel predecessors. Consequently, the use of biofuels contribute to the realization of Sustainable Development

Goal 7 (SDG 7) which aims to ensure affordable, reliable, sustainable and modern energy for all and SDG 13, that calls for urgent action to combat climate change and its effects [6–8].

The predominant forms of biofuels are gaseous, solid or liquid depending on the biomass source and the conversion process. Primary biofuels such as fuel wood, wood pellets and briquettes are organic materials used in their unprocessed natural form whose energy is released through direct combustion while secondary biofuels such as bioethanol, biodiesel and biogas are produced through the thermo-chemical or biochemical conversion of biomass or other organic materials like wastes. The secondary biofuels can be categorized into four generations based on the source of the biomass and production technology. First generation biofuels are biofuels produced from food crops like corn and sugarcane for ethanol, and vegetable oils or animal fats for biodiesel. This type of biofuels offers benefits such as high-octane ratings, reduced emissions and require simple biochemical treatments for conversion to transportation fuels. Second-generation biofuels are fuels made from lignocellulosic or woody biomass, or agricultural residues. Third-generation biofuels are algae-based biofuels, where algae are harvested to produce oil, which is then converted into biodiesel. Algae grow quickly and do not require pretreatment, but controlling the environment for optimal growth can be challenging and expensive. Fourth generation biofuels are the latest biofuels from genetically modified organisms. They encompass combined advanced bioengineering to increase the desired traits of organisms used in biofuel production. Fourth-generation biofuels offer significant potential for the biofuel industry, but require further advancements in scaling up production and reducing costs for their successful commercialization [9]. Biofuels are produced from a wide variety of feedstock sources thus showcasing the diversity of biomass resources. This minimizes dependency on a single crop feedstock, hence promoting agricultural sustainability.

Biofuels such as biodiesel, bioethanol and biogas have drawn attention from the world as viable alternative sources of petroleum-derived fuels [10,11]. Biodiesel is a renewable, low-carbon, clean-burning fuel produced through the transesterification process using feedstocks such as vegetable oil or animal fats. Biodiesel is a high oxygen fuel that can be blended with diesel at any ratio (without the need of engine modifications) to improve its octane rating, combustion efficiency and reduce green-house gas emissions [12]. This allows for a smooth transition to cleaner energy without requiring complex engine modifications. The usage of biodiesel will therefore minimise air pollutants such as hydrocarbons, carbon monoxide and particulate matter. Additionally, biodiesel has a higher cetane number than petroleum diesel thus improving ignition and combustion efficiency when combined with petroleum diesel. Biodiesel has the potential for carbon neutrality, due to balance between the amount of CO_2 emissions and the amount of CO_2 absorbed by the plants producing vegetable oil being equal [13].

Biogas is a gaseous biofuel produced through fermentation of organic matter such as livestock manure, municipal solid waste or weeds through anaerobic digestion using microorganisms. The raw materials are readily available and cheap. Biogas which contains methane, carbon dioxide and traces of hydrogen sulphide, can be refined into biomethane, which serves as a clean source for heat and power generation, as well as for producing renewable fuels and chemicals. Biogas has traditionally been used for direct combustion in cooking and lighting. In recent years, its use for electricity generation has grown in many countries. Biogas-powered electricity systems can operate both off-grid and on-grid, making biogas a suitable option for decentralized energy production [9,14].

Although biogas is an important decentralized energy resource, its combustion chemistry is inherently complex due to significant CO_2 dilution [15]. CO_2 acts both as a thermal diluent and influences the radical chemistry by modifying radical concentrations and increasing ignition delay times. This underscores the need to systematically assess chemical enhancement approaches, such as hydrogen enrichment, to improve combustion performance.

Bioethanol is another vital biofuel; it represents 82% of the total biofuels produced. Bioethanol is produced from the fermentation of different feedstock such as sugar and starch crops such as corn. More recently, it is produced from microalgae. It is one of the preferred biofuels to replace fossil fuels, because its sources are renewable, it has high octane-number rating, it is environmentally friendly and it is like gasoline, so its use does not require engine modification.

Unlike traditional hydrocarbon streams, the combustion chemistry of bioethanol is fundamentally dictated by its high fuel-bound oxygen content and low energy density. While its elevated heat of vaporization improves engine knock resistance, its chemical kinetic profile exhibits a highly unique, less pronounced negative temperature coefficient (NTC) behavior in the intermediate temperature range (700–900K) compared to gasoline [16]. This structural variance alters the intermediate radical pool during low-temperature oxidation, suppressing polycyclic aromatic hydrocarbon (PAH) soot precursors but initiating a competing pathway that accelerates toxic aldehyde and unburned oxygenate emissions. Consequently, guiding the field requires isolating the specific chemical kinetic mechanisms that govern these non-linear radical interactions, particularly when bioethanol is blended with fossil fuels, to optimize advanced low-temperature combustion (LTC) regimes.

1.2. Current Challenges in Biofuel Utilization

Despite their significant potential, biofuels face major challenges relating to feedstock supply, production economics, fuel properties, and emissions performance. Biofuels are in competition for raw materials also with other industries [17]. From this viewpoint, a careful monitoring of biofuel demand impact on other markets is considered.

Production of biofuels from lignocellulosic biomass via biochemical and thermochemical pathways has its own challenges. Major technical challenges and barriers to the biochemical pathway include dealing with the variability of biomass feedstocks, general recalcitrance of lignocellulosic materials to chemical and/or biological degradation, and the need for improved effectiveness of cellulose enzymes and fermentation organisms [18,19]. For thermochemical approaches (gasification and pyrolysis), pre-treatment of the biomass and physical feeding into thermal processing units are challenging [20].

The major issue with biodiesel utilization is the limited availability and high cost of feedstocks, which contribute up to 75% of total production costs [21]. Reliance on edible oils like palm or soybean raises the food versus fuel debate, whereas using alternative feedstocks such as waste vegetable oil or non-edible oils from plants such as jatropha, jojoba, algae and animal tallow castor can help lower production expenses [22]. However, many of these alternative sources are still underdeveloped at a commercial scale. Technical challenges of biodiesel include lower calorific value, higher viscosity, and density than that of conventional diesel, which lead to increased fuel consumption and potential problems in engine injection and atomization systems. Slight reductions in engine power and thermal efficiency have been reported with its use [23]. Additionally, biodiesel tends to cause slight decreases in power output and increases in NO_x emissions compared to fossil diesel.

Bioethanol has a lower energy content compared to fossil fuels. For example, one gallon of ethanol produces less energy than one gallon of gasoline, resulting in reduced fuel efficiency [13]. Additionally, ethanol produced from corn is neither cheaper nor extremely pure from the standpoint of environmental protection and requires higher energy consumption to be processed.

The IEA Outlook for Biogas and Biomethane points out that while biogas has strong potential for decarbonization and energy security, its utilization faces persistent challenges. These include feedstock variability and unreliable supply chains, methane leakage risks that undermine climate benefits, and the high costs of upgrading biogas to biomethane, which make it less competitive than fossil natural gas [24]. Biogas also faces combustion challenges due to impurities and compositional variability [25].

1.3. Scope and Objectives of the Study

The present study provides a comprehensive overview of recent advancements in biofuel combustion chemistry. The study provides a comprehensive review of the fundamental chemical properties of common biofuels (biodiesel, bioethanol, and biogas), and an exploration of combustion mechanisms. It critically evaluates the recent works in both experimental diagnostic tools and computational modeling techniques that have significantly enhanced our ability to study these complex processes. The novelty of the present study lies in the concise review of biofuels with a critical evaluation of the combustion kinetics and mechanisms. The potential of various biofuels as well as blending of biofuels is critically reviewed. The study identifies challenges limiting the application of biofuels and proposes solutions, highlights future areas of study and opportunities in this rapidly evolving field. As such, the study synthesizes current knowledge to inform future research and development efforts aimed at optimizing biofuel combustion for cleaner and more efficient energy conversion.

2. Fundamentals of Biofuel Combustion

Biofuel combustion is the thermo-chemical process through which bio-derived fuels such as bioethanol, biogas and biodiesel combine with oxygen in a high temperature environment producing energy in the form of heat, carbon dioxide and water vapour. The fundamentals of biofuel combustion are grounded in their different chemical compositions such as the long-chain hydrocarbons in biodiesel, short carbon chain with high oxygen content in bioethanol and the methane-carbon dioxide blend in biogas. These diverse chemical compositions in biofuels determine their combustion characteristics.

2.1. Chemical composition of common biofuels

Biodiesel is primarily composed of monoalkyl esters of long chain fatty acid mainly methyl or ethyl esters (FAMEs), which are produced through the process of transesterification. This process involves a reaction between renewable lipids such as plant oils or animal fats and methanol (or ethanol) in the presence of a catalyst (typically sodium or potassium hydroxide). The general formula for biodiesel is $R\text{-}COOCH_3$, where R is a long hydrocarbon

chain (between C_{16}–C_{22}). The fatty acid composition such as the chain length and degree of unsaturation varies depending on the feedstock used such as rapeseed, soybean or palm oils. Biodiesel mainly comprises five components: methyl palmitate ($C_{17}H_{34}O_2$), methyl stearate ($C_{19}H_{38}O_2$), methyl oleate ($C_{19}H_{36}O_2$), methyl linoleate ($C_{19}H_{34}O_2$), and methyl linolenate ($C_{19}H_{32}O_2$) [26].

The stoichiometric combustion equation for a representative biodiesel compound such as $C_{17}H_{34}O_2$, which approximates a common fatty acid methyl ester like methyl palmitate can be expressed as follows when reacting with oxygen:

$$C_{17}H_{34}O_2+25.5O_2 \rightarrow 17CO_2+17H_2O \quad (1)$$

The molecular structure of fatty acid esters, defined by carbon chain length, saturation level, and functional groups in fatty acid esters directly affects biodiesel performance properties such as cold flow behavior (such as pour and cloud points), density and viscosity, cetane number, oxidation stability, and calorific value [27,28].

Bioethanol, a simple alcohol with the chemical formula C_2H_5OH, consists of carbon (C), hydrogen (H), and oxygen (O), and is typically produced through the fermentation of sugars or starches from biomass. The presence of an oxygen atom within its molecular structure distinguishes bioethanol from many hydrocarbon fuels, contributing to its relatively clean-burning nature. During combustion, bioethanol reacts with oxygen to form carbon dioxide and water:

$$C_2H_5OH + 3O_2 \rightarrow 2CO_2+3H_2O \quad (2)$$

The oxygen content in ethanol facilitates more complete combustion, resulting in lower emissions of carbon monoxide (CO), unburned hydrocarbons, and particulates compared to traditional gasoline. Additionally, bioethanol has a high-octane number and vaporization heat, which enhances knock resistance in engines. However, it has a lower energy density (around 50% that of gasoline), therefore more volume is required to produce the same amount of energy [29].

Biogas is a gaseous mixture primarily composed of methane (CH_4) and carbon dioxide (CO_2), with small amounts of hydrogen sulfide (H_2S), hydrogen (H_2), nitrogen (N_2), and trace moisture. Its composition depends on the feedstock and the anaerobic digestion process used. A typical biogas mixture contains 50–70% CH_4 and 30–50% CO_2 [30]. The methane component is the primary combustible element and is responsible for the energy content of biogas while, carbon dioxide is the main non-combustible constituent of biogas that lowers its overall calorific value through a dilution effect. This results to several operational challenges, including reduced flame stability, higher flame extinction limits and poor combustion control. In addition, the presence of CO_2 complicates the understanding of emission formation mechanisms[31,32].

The combustion of methane occurs via the reaction:

$$CH_4+2O_2 \rightarrow CO_2+2H_2O \quad (3)$$

The high methane content allows biogas to burn efficiently with a clean blue flame when properly combusted. The main impurities are carbon dioxide, which lowers the energy content of the gas and hydrogen sulphide which could cause corrosion problems on engine parts and on human health. Therefore, biogas purification (upgrading) is necessary especially when used in engines or for grid injection [33]. Purified biogas (biomethane), can then mimic the combustion behavior of natural gas more closely, offering stable flame characteristics and higher efficiency. The physical and chemical properties of biofuels are shown in Table 1.

2.2. Comparison with Traditional Fossil Fuels

Fossil fuels and biofuels represent distinct categories of energy sources with significant differences in their origin, environmental impact, and sustainability. Fossil fuels, such as coal, oil, and natural gas, were formed from the anaerobic decomposition of ancient organic matter over millions of years, making them finite, non-renewable resources. Biofuels on the other hand are derived from renewable materials. Table 2 shows the main differences between fossil fuels and biofuels.

Table 1. Physical and chemical properties of biofuels [26–34].

	Physical Properties					Chemical Properties						
	Density (at 15 °C)	**Boiling Point**	**Viscosity**	**Flash Point**	**Heating Value**	**Chemical Formula**	**Molecular Weight**	**LHV**	**HHV**	**Octane Number**	**Cetane Number**	**Autoignition Temperature**
Bioethanol	789 kg/m^3	78.4 °C	1.2–1.5 cSt (or mm^2/s) (at 20 °C)	12 °C	6380kcal/kg	C_2H_5OH	46.07 g/mol	26.3 MJ/kg	29.1 MJ/kg	108–110	5.8	425 °C
Biodiesel	860–900 kg/m^3	>300 °C	3.6–6 mm^2/s (at 40 °C)	>147 °C	39–41MJ/kg	Approx. C_{16}–$C_{18}H_{32-36}O_2$ (FAMEs)	270–319 g/mol	39 MJ/kg	42 MJ/kg	N/A	48–65	256–330 °C
Biogas	1.2 kg/m^3	-	11–13 µPa.s at 0 °C	−188 °C	22MJ/m^3	Mainly CH_4, H_2S & CO_2	22–26 g/mol	22 MJ/m^3	25 MJ/m^3	120–130	<5	540–600 °C

Table 2. Characteristics of fossil fuels and biofuels.

Characteristic	Fossil Fuels	Biofuels	Ref
Carbon neutrality	Increases the concentration of carbon dioxide in the atmosphere	Releases net zero carbon dioxide into the atmosphere	[35]
Efficiency	High efficiency levels in internal combustion engines, particularly in well-optimized gasoline and diesel engines.	The efficiency of engines running on biofuels can vary depending on factors such as fuel composition, engine design, and operating conditions	[36]
Energy density	Produces a high amount of energy per unit mass	Produces a low amount of energy per unit biomass	[37]
Toxicity	Toxic ingredients, chemicals and by-products	Non-toxic	[37,38]
Environmentally friendly	No due to high emissions of CO, nitrogen oxides (NO_x), and volatile organic compounds (VOCs) compared to biofuels. This leads to air pollution and smog formation	Yes. Bioethanol and biodiesel typically produce lower levels of carbon monoxide (CO), particulate matter (PM), and sulfur oxides (SO_x) during combustion, contributing to cleaner air quality and reduced environmental impact.	[39]
Production methods	Extracted from fossil reserves through drilling, mining, or extraction processes	Bioethanol through fermentation, biodiesel through transesterification, biogas through anaerobic digestion of organic matter	[40]
Affordability	Expensive due to non-renewability of the sources	Biomass raw materials are readily available hence cheap	

2.3. Basic Combustion Mechanisms and Kinetics

Biodiesel, composed mainly of fatty acid methyl esters (FAMEs), undergoes combustion in compression ignition engines through a series of physical and chemical processes. The combustion pathway is complex due to the molecular structure of FAMEs, which includes long hydrocarbon chains and oxygen-containing ester groups. The combustion mechanism of biodiesel involves the following four steps: Fuel pyrolysis, radical formation, chain branching to final combustion [41]:

Pyrolysis occurs at temperatures above 600–1000 °C where biodiesel molecules start to thermally break down into smaller hydrocarbons, aldehydes, alkenes, and radicals.

$$C_{17}H_{34}O_2 \text{ (Methyl palmitate)} \rightarrow C_8H_{16} + C_9H_{18} + CO + CO_2 + H_2O + \text{radicals} \quad (4)$$

Radicals (R•) react with O_2 to form intermediate species (alkylperoxy radicals) (ROO•). These species further undergo isomerization and chain branching, especially at low temperatures. In the high-temperature combustion zone, the remaining intermediates are fully oxidized to carbon dioxide and water as represented in Equation (1), with minor emissions of NO_x and CO.

The combustion characteristics of biodiesel and its blends with petroleum diesel are strongly governed by feedstock-dependent FAME composition, oxygen content, and blend ratio. At the droplet scale, the steady combustion rate increases linearly with biodiesel concentration due to biodiesel's oxygenated nature, which enhances oxidation efficiency. Lower blends (B5–B25) behave more like diesel but show strong puffing and micro-explosions that improve atomization, while higher blends (B50–B75) burn more steadily due to higher oxygen content but evaporate more slowly and have longer ignition delays. Saturated-rich biodiesels from waste cooking oil and animal fats tend to form more soot and ignite later, whereas unsaturated-rich biodiesels burn cleaner with better atomization [42]. Optimizing biodiesel blends is essential to balance ignition stability, combustion efficiency, and emissions control.

Bioethanol combustion follows these general steps: Fuel decomposition, Radical reactions, chain branching to final combustion [43]. Equations (5) and (6) represent the initial and final combustion reactions.

$$C_2H_5OH \rightarrow CH_3\bullet + CH_2OH\bullet \quad (5)$$

$$CO + OH \rightarrow CO_2 + H \quad (6)$$

Ethanol has a shorter ignition delay than gasoline, due to its oxygen content, which facilitates faster combustion reactions. It also promotes cleaner combustion with significantly less soot formation compared to gasoline, although it produces aldehydes as intermediate species during the oxidation step [44]. Ethanol has a higher laminar flame speed, making it suitable for use in spark-ignition engines [45].

Figure 1 shows the combustion mechanisms for biofuels.

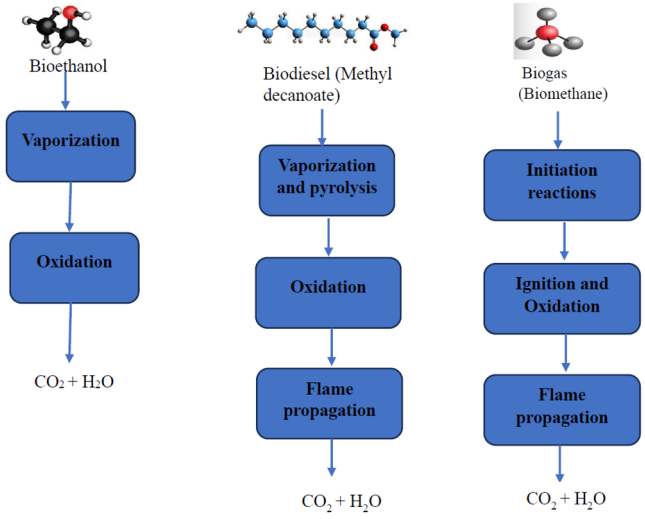

Figure 1. Combustion mechanisms of biofuels.

The combustion characteristics of biogas are dependent on the methane content which provides the energy for combustion. CO_2 acts as a diluent which lowers the flame temperature. The low calorific value of biogas can be improved through addition of hydrogen. Combustion of biogas follows radical chain reactions as follows: Initial

reactions; At high temperatures stable methane molecules begin to break to form free radicals. Propagation reactions: These initial free radicals attack the fuel and oxidant molecules, creating more products and radicals, thus propagating the chain reaction. Chain branching and termination; These are reactions that produce more radicals which are highly reactive, leading to an exponential increase in the reaction rate and the phenomenon of ignition.

In the analysis of biogas combustion, researchers mainly focus on its two primary components. The combustion of a methane and carbon dioxide mixture serves as a representative model for the overall process. A mixture of 60% CH_4 and 40% CO_2 reacting with air is assumed to depict typical biogas combustion. Equations (7) and (8) represent the combustion of pure methane in oxygen and biogas in air, respectively [46,47]:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{7}$$

$$0.6CH_4 + 0.4CO_2 + 1.2(O_2 + 3.76N_2) \rightarrow CO_2 + 1.2H_2O + 4.512N_2 \tag{8}$$

Biogas combustion kinetics examine the rate at which chemical reactions occur and the variables that influence these reaction rates. The main factors affecting combustion rates include temperature, pressure, and reactant concentrations [48]. The relationship between temperature and reaction rate is commonly described by the Arrhenius equation:

$$k = A^{e-Ea/RT} \tag{9}$$

where k is the rate constant, A denotes the pre-exponential factor, E_a is the activation energy, R is the universal gas constant, and T is the absolute temperature.

Table 3 show a comparison of the combustion and kinetic parameters of bioethanol, biodiesel and biogas.

Table 3. Comparative analysis of fundamental combustion and kinetic parameters for bioethanol, biodiesel, and biogas.

Fuel Property	Bioethanol	Biodiesel	Biogas	References
Laminar Flame speed	High (40–50 cm/s at 1atm, 360 K	Low to Moderate (21–25 cm/s at 1atm, 400 K	Low (21–29.5) cm/s at 0.28 atm, 295 K heavily suppressed by dilution	[49–51]
Ignition Delay Time (IDT) Regimes	Exhibits distinct Negative Temperature Coefficient (NTC) behavior at intermediate temperatures (700–900 K)	Short IDT; highly reactive at low temperatures; NTC behaviour is heavily suppressed due to long alkyl chains	Significantly prolonged IDT due to the thermal and chemical third-body effects of CO_2	[52–54]
Dominant Intermediate Species	Formaldehyde (HCHO) Acetaldehyde (CH_3CHO) and Ethene (C_2H_4)	Alkyl radicals, Ester-group intermediates, Propene, Olefins	Methyl radicals (CH_3), Formyl radicals (HCO), Carbon monoxide (CO)	[55–57]
Key Kinetic Pathways	Focuses on radical driven decomposition where, OH, H, and O radicals react by stripping hydrogen atoms (H-abstraction)	Fuel oxidation shifts from low-temperature peroxy radical to high-temperature β-scission of long hydrocarbon chains; (RO_2) isomerization	$CH_4 + OH \rightarrow CH_3 + H_2O$ followed by slow, rate-limiting CO oxidation $CO + OH \rightarrow CO_2 + H$	[58,59]
Primary Emission Trade-offs	Low soot and Polycyclic Aromatic Hydrocarbon (PAH) formation; risk of unburned aldehyde emissions	High Soot-NO_x trade-off; due to higher combustion temperatures and oxygen availability	Lower flame temperatures generally reduce thermal NO_x due to reduced peak flame temperatures; elevated incomplete CO emissions under lean conditions	[60]

3. Advances in Experimental Techniques

3.1. Development of Advanced Diagnostic Tools

The development of sustainable and efficient combustion systems for biofuels demands a deep understanding of their underlying chemical kinetics and reaction pathways. Traditional diagnostic techniques often lacked the resolution, sensitivity, or temporal fidelity required to track fast, transient species in combustion environments. In recent years, spectroscopy and mass spectrometry have emerged as indispensable tools in combustion diagnostics, enabling researchers to probe the complex chemistry of biofuels at molecular levels [61]. Table 4 shows the comparative analysis of different diagnostic techniques, their strengths and limitations.

3.1.1. Spectroscopy

Spectroscopy entails the study of the interaction between electromagnetic radiation and matter. In combustion chemistry, spectroscopy is used to identify and quantify reactive intermediates, stable products, and radicals formed during fuel decomposition and oxidation. These measurements are essential for validating chemical kinetic models and optimizing combustion conditions. Biofuels like ethanol, butanol, biodiesel, and other oxygenated fuels tend to have unique decomposition pathways that produce oxygenates, aldehydes, and radicals not commonly observed in hydrocarbon fuel combustion. Spectroscopic diagnostics enable the capture of these unique signatures and support the

development of fuel-specific kinetic models. Examples of spectroscopic diagnostics include Laser-based spectroscopy, UV-VIS absorption spectroscopy and Raman spectroscopy. Their operations are discussed further below.

(a) Laser-Based Spectroscopy

Techniques such as Laser-Induced Fluorescence (LIF) and Raman/Rayleigh scattering have become very useful diagnostic tools. LIF allows for the highly sensitive detection of specific, short-lived radical species like hydroxyl (OH) and formaldehyde (CH_2O), which are crucial intermediates in combustion. By exciting a target molecule with a laser and measuring the emitted fluorescence, researchers can map its concentration in both space and time within a flame or reactor [62]. This is useful for characterizing complex biofuel mixtures, such as fuel/water emulsions with ethanol [63]. A study done by [64] developed a technique that uses a single femtosecond laser pulse to simultaneously detect NO_x, O, and O_2 in flames. The method delivered accurate, interference-free results that matched with simulation data, providing valuable insights for species distribution and the pathways of NO_x formation in both lean and rich combustion environments. Advanced techniques like two-photon LIF enable the detection of atoms like hydrogen and oxygen. Raman and Rayleigh scattering are used to measure the temperature and the concentration of major species (like O_2, N_2, CO_2, H_2O) by analyzing how light scatters off molecules [65].

(b) Ultraviolet and Visible Absorption Spectroscopy

UV-Vis absorption spectroscopy operates on the principle that specific molecules absorb light within the ultraviolet (100–400 nm) and visible (400–700 nm) regions of the electromagnetic spectrum as their electrons transition to higher energy levels. The extent of this absorption is directly proportional to the concentration of the absorbing species. In the context of biofuel combustion, this technique is particularly effective for detecting and quantifying gaseous pollutants such as nitric oxide (NO) and nitrogen dioxide (NO_2), both are significant contributors to NO_x emissions [66]. By monitoring their characteristic absorption bands, researchers can assess the effectiveness of different combustion strategies in mitigating these harmful byproducts. Furthermore, UV-Vis spectroscopy plays an important role in identifying and quantifying aromatic intermediates and soot precursors, like polycyclic aromatic hydrocarbons (PAHs), which are formed during incomplete biofuel combustion [67]. Many of these aromatic compounds absorb strongly in the UV region thus allowing for their identification and analysis. Beyond the combustion process itself, UV-Vis can also be employed for biofuel quality assessment, such as determining blend levels of biodiesel in conventional diesel or monitoring the oxidative degradation of biofuels [68]. While relatively simple and cost-effective, limitations include potential interferences from overlapping absorption spectra in complex combustion environments and the inability to directly detect non-absorbing major species like oxygen or nitrogen.

(c) Raman spectroscopy

Raman spectroscopy, a non-intrusive vibrational spectroscopic technique, complements UV-Vis by providing information on the molecular vibrations of a sample [69]. It is an effective tool in optimizing combustion processes that works by analyzing the inelastic scattering of monochromatic light (typically from a laser) from molecules, revealing a unique spectral fingerprint for each species. A significant advantage of Raman spectroscopy in biofuel combustion is its ability to detect major species that are often transparent to UV-Vis, including homonuclear diatomic molecules like hydrogen (H_2), oxygen (O_2), and nitrogen (N_2), as well as heteronuclear molecules such as carbon dioxide (CO_2) and methane (CH_2) [70]. This capability is fundamental for understanding the overall stoichiometry and progression of reactions within biofuel flames, allowing for quantification of these critical components. Moreover, Raman spectroscopy is a powerful tool for measuring temperature fields within combustion zones. The sensitivity of Raman band intensities and distributions to temperature allows for precise local temperature determinations, which are vital for understanding reaction kinetics and optimizing combustion efficiency. The technique also excels at characterizing fuel-air mixing, an essential parameter for clean and efficient combustion, by measuring the concentrations of fuel and oxidizer components. Recent advancements have significantly improved signal-to-noise ratios and acquisition speeds, enabling real-time diagnostics even in highly turbulent biofuel flames [71]. This breakthrough is critical for deciphering the intricate interactions between turbulence and chemical reactions, paving the way for more accurate combustion models. Furthermore, Raman spectroscopy is widely used for characterizing the structure and defects of soot, providing insights into particulate matter emissions from biofuels [72]. Despite its power, Raman spectroscopy faces challenges such as the inherent weakness of the Raman signal, potential fluorescence interference, and the relatively higher cost and complexity of the instrumentation.

3.1.2. Mass Spectrometry

Mass spectrometry (MS) is a powerful diagnostic tool in combustion research, offering high sensitivity and specificity for detecting a wide range of species, including transient intermediates and stable products. In the context of biofuels combustion, MS plays a crucial role in unraveling complex reaction mechanisms, especially

given the diverse chemical structures and oxygenated nature of many biofuels [73]. The two major MS techniques are: Molecular beam mass spectrometry (MBMS) and Photoionization mass spectrometry (PIMS). Molecular beam mass spectrometry (MBMS**)** is widely used to sample combustion gases directly from flames or shock tubes. By rapidly expanding the sample into a vacuum, MBMS minimizes secondary reactions and allows for real-time detection of reactive intermediates such as radicals, aldehydes, and hydroperoxides. This is particularly important for studying ignition behavior and pollutant formation in alcohols, esters, and other biofuel types. Photoionization mass spectrometry (PIMS**)** has further advanced combustion diagnostics by using soft ionization methods that reduce molecular fragmentation. This enables the identification of larger and more fragile species, including isomers and complex intermediates found in the combustion of lignocellulosic or furan-based biofuels. PIMS offers rapid, high-resolution detection across a broad mass range [74]. Overall, mass spectrometry has become essential for investigating the combustion chemistry of biofuels. It supports the validation of reaction mechanisms, optimization of combustion systems, and reduction of emissions, making it a key component in the development of cleaner and more efficient biofuel technologies [75].

3.2. Microkinetic Experiments and Reactor Studies

Microkinetic experiments and reactor studies are crucial in the development and optimization of biofuel production processes. The microkinetic experiments enable understanding fundamental reaction mechanisms by determining the reaction intermediate and rate-determining steps. As such, they are essential for catalyst design and optimization by identifying the optimal catalyst composition and structure to maximize reaction rate and selectivity. The microkinetic studies are done using Shock Tubes and Rapid Compression Machines (RCMs) or Flow and Jet-Stirred Reactors (JSRs).

The Shock Tubes and Rapid Compression Machines (RCMs) are the primary tools for studying gas-phase chemical kinetics at high temperatures and pressures relevant to internal combustion engines. A shock tube uses a shock wave to nearly instantaneously heat a gas mixture, allowing for the measurement of ignition delay times and species concentration profiles over very short timescales. RCMs compress a gas mixture to simulate compression stroke of an engine. Both methods provide high-quality data for fundamental kinetic parameters, such as the ignition delay of fuels like rapeseed oil and ethanol emulsions [76], under conditions where the complexities of fluid dynamics are minimized.

The Flow and Jet-Stirred Reactors (JSRs) are used for studying kinetics over longer timescales and at more moderate conditions and flow reactors and JSRs are employed. In a JSR, reactants are continuously fed into a vessel in which intense mixing creates a uniform environment. By analyzing the composition of the outflowing gas at steady state, researchers can obtain data on the reaction rates and the formation of various intermediate products and pollutants. These reactors are crucial for understanding the low-to-intermediate temperature chemistry that governs phenomena like autoignition and the formation of soot precursors from various biofuel candidates [77].

3.3. Flame Characterization Techniques

Flame characterization techniques for biofuels involve various methods to understand their combustion properties and emissions. Key aspects include temperature, species distribution, soot formation, and pollutant emissions. The main flame characterization techniques include:

(a) Flame Speed Measurements

The laminar flame speed is a fundamental property of a fuel-air mixture that quantifies its reactivity. Techniques for measuring it, such as the counterflow flame and spherically expanding flame methods, have been refined for higher accuracy. These measurements provide key validation targets for chemical kinetic models of a wide range of biofuels, including gasoline/alcohol blends [78].

(b) Species and Temperature Mapping in Flames

Combining laser diagnostics with various flame setups allows for detailed mapping of flame structure. For example, using LIF to measure OH concentration across a flame front provides insight into the primary reaction zone. Coherent Anti-Stokes Raman Spectroscopy (CARS) is an advanced technique used for making precise, spatially resolved temperature measurements within flames. Particle Image Velocimetry (PIV) is used to measure the velocity field of the unburned and burned gases, providing crucial information about the fluid dynamics and its interaction with the flame chemistry [79].

Table 4. Comparative analysis of advanced experimental techniques, strengths and weaknesses.

Experimental Technique	Principle	Key Measured Outputs	Bioethanol Relevance	Biodiesel Relevance	Biogas Relevance	Strengths	Limitations	Ref
Laser-based spectroscopy (LIF/PLIF)	Laser excitation of molecules fluorescence emission	Radical species (OH, CH, CH_2O), flame structure	Tracks ethanol oxidation pathways and intermediate species formation	Identifies soot precursors and local oxidation zones in FAME combustion	Captures flame stability in CH_4/CO_2-diluted mixtures	High spatial/temporal resolution; non-intrusive	Expensive; requires complex calibration	[80,81]
UV–Vis absorption spectroscopy	Absorption of UV/visible light by gas-phase species	CO, NO, NO_2 and formaldehyde concentrations	Useful for CO/NO_x formation trends during alcohol combustion	Tracks NO_x formation under oxygenated fuel conditions	Measures CO_2 dilution and incomplete combustion products	Simple setup; real-time monitoring	Limited species selectivity; line-of-sight averaging	[82]
Raman spectroscopy	Inelastic scattering of laser light	Temperature, major species (CH_4, O_2, CO_2, H_2O)	Maps temperature and fuel decomposition pathways	Tracks oxygenated fuel breakdown and oxidation completeness	Strong for CH_4–CO_2 mixture composition and temperature fields	Simultaneous species temperature data	Weak signal; sensitive to noise	[83]
Mass spectrometry (MBMS, molecular beam MS)	Ionization and separation of gas-phase species by mass/charge ratio	Intermediates, radicals, reaction products	Captures ethanol, acetaldehyde and CO_2 pathways	Resolves complex biodiesel (FAME) breakdown chemistry	Detects methane oxidation intermediates	Highly detailed chemical speciation	Expensive; intrusive sampling	[84]
Microkinetic/reactor studies	Controlled reactors and kinetic modelling	Reaction rates, rate constants, mechanism validation	Validates alcohol oxidation mechanisms	Essential for multi-step FAME oxidation networks	Used for methane oxidation kinetics under dilution effects	Strong for model development	Limited flame realism (compared to real flames)	[85]
Laminar flame speed measurements	Observation of planar flame propagation	Flame speed, flame stability limits	High flame speed due to oxygen content	Moderate flame speeds influenced by heavier molecules	Low flame speed due to CO_2 dilution	Direct combustion performance indicator	Sensitive to conditions (T, P, φ)	[86,87]

4. Advances in Computational Modeling

Alongside experimental progress, computational modeling has become an essential tool for interpreting experimental data and predicting combustion behavior. Advances in computational modeling have enabled the accurate prediction of key processes such as atomization, and combustion of biofuels.

4.1. Factors Affecting Computational Modeling of Biofuels

Detailed kinetic models are the cornerstone of predictive combustion simulation. They consist of a comprehensive set of elementary chemical reactions, their corresponding rate constants, and the thermochemical and transport properties of all species involved. This section presents factors affecting computational modeling of biofuels.

(a) Mechanism complexity

One of the main challenges in computational modelling of biofuel combustion is the complexity of the chemical kinetic mechanisms of biofuels. While conventional hydrocarbon fuels are often represented using relatively compact reaction schemes, biofuels contain oxygenated functional groups and diverse molecular structures that substantially increase the number of reaction pathways. For example, a model for methane might contain a few hundred reactions, whereas a model for a biodiesel surrogate can involve thousands of species and tens of thousands of reactions. Identifying the key kinetic steps in these large mechanisms is a major focus of modern research [88]. Increasing mechanism complexity improves predictive accuracy for ignition delay, flame speed, and pollutant formation but at the expense of computational efficiency [89].

(b) Automated mechanism generation

To handle mechanism complexity, researchers increasingly rely on automated reaction mechanism generation software. These programs use a set of predefined reaction family rules to systematically build a network of all possible reactions starting from the initial fuel molecules. This automates the previously painstaking manual process and helps ensure that no important reaction pathways are overlooked [90]. Despite these advances, automated mechanisms frequently produce excessively large reaction networks, creating challenges in model validation and computational manageability. Furthermore, generated mechanisms often depend on estimated thermodynamic and kinetic parameters, introducing uncertainties that propagate into combustion simulations. Several recent studies have emphasized the need for uncertainty quantification frameworks alongside automated generation procedures [91].

(c) Quantum chemistry for parameterization

The accuracy of a kinetic model depends entirely on the accuracy of its input parameters, namely reaction rate constants and thermochemical properties. For many biofuel-specific intermediates, this data does not exist experimentally. Modern computational chemistry, particularly high-level quantum mechanical calculations, has become the primary source for this data [92]. These first principles calculations can predict the energetic barriers of reactions and the properties of molecules with high accuracy, providing the essential data needed to build reliable models [93].

(d) Model reduction

While detailed models are essential for accuracy, their large size makes them computationally too expensive for use in complex fluid dynamics simulations. Therefore, a critical step is mechanism reduction, where systematic techniques are used to eliminate unimportant species and reactions. This creates a smaller, computationally tractable model that still accurately reproduces the key combustion targets such as ignition delay and flame speed of the detailed mechanism [94].

4.2. Quantum Chemical Calculations for Reaction Pathways

Beyond providing parameters, quantum chemistry is used to explore entire reaction pathways for biofuel molecules. By mapping the potential energy surface (PES) for the decomposition and oxidation of a fuel [95], researchers can identify novel, previously unknown reaction channels. This is especially important for oxygenated biofuels, whose functional groups (like esters, alcohols, or furans) introduce reaction pathways that are not present in traditional hydrocarbon fuels. For example, detailed PES studies have revealed unique decomposition routes for methyl esters (a key component of biodiesel) and have clarified the complex chemistry of furanic compounds, which are promising second-generation biofuels. These theoretical insights guide the development of more accurate and comprehensive kinetic mechanisms [96].

4.3. Large-Scale Simulations

To bridge the gap between fundamental chemical kinetics and real-world combustion devices, large-scale computational fluid dynamics (CFD) simulations are employed. Some of the major CFD simulations are discussed further.

(a) Direct Numerical Simulation (DNS)

DNS is the most detailed type of CFD simulation, as it resolves all scales of turbulent motion and directly incorporates detailed chemical kinetic models. While computationally prohibitive for full-scale engine simulations, DNS is an invaluable research tool. It provides a 'numerical experiment' that yields complete, time-resolved data for velocities, temperatures, and species concentrations throughout the simulation domain. DNS of turbulent flames fueled by biofuels like ethanol have provided fundamental insights into turbulence-chemistry interactions [97], pollutant formation, and autoignition phenomena under engine-relevant conditions.

(b) Large Eddy Simulation (LES)

LES is a more practical approach for simulating realistic combustors. It directly computes the large, energy-carrying turbulent eddies while modeling the effects of the smaller, more universal scales. When combined with reduced chemical kinetic mechanisms, LES can predict the performance and emissions of internal combustion engines, gas turbines, and industrial burners. Recent advances in computing power and modeling techniques have enabled high-fidelity LES of biofuel combustion in complex engine geometries, helping to optimize engine design and control strategies for alternative fuels [98].

4.4. Machine Learning Applications in Combustion Chemistry

The vast amount of data generated from both experiments and high-fidelity simulations has paved the way for the application of machine learning (ML). As such, there is an increasing application of ML in combustion chemistry aimed at improving the accuracy and efficiency of experimental studies and simulations. Typical applications and benefits of ML techniques are discussed in this section.

(a) Accelerating Quantum Chemistry

ML models can be trained on datasets of quantum chemical calculations to predict molecular properties and reaction energies at a fraction of the computational cost. This accelerates the process of parameterizing kinetic models for new biofuel candidates [99]. It therefore reduces the computational cost of complex combustion simulations.

(b) Mechanism Reduction and Optimization

ML techniques, such as neural networks and genetic algorithms, are being used to automate and improve the process of chemical mechanism reduction. These methods can identify the most important reactions and species more efficiently than traditional techniques, leading to compact and accurate models suitable for computational fluid dynamics [100]. This also accelerates chemical kinetics calculations.

(c) Surrogate Model Development

For complex real-world simulations, machine learning (ML) can be used to create surrogate models, also known as response surfaces, that emulate the behavior of a detailed combustion simulation. These fast-running surrogates can then be used for large-scale design optimization and uncertainty quantification studies, significantly reducing the computational turnaround time [101]. In addition, the application of ML aids the development of more accurate models for turbulent combustion. This further helps to analyze large datasets, identify hidden patterns and relationships under various conditions. Data availability remains a major drawback since many surrogate models are trained on synthetic datasets that may not adequately represent practical combustion conditions [102].

5. Assessment of Biofuel Combustion

In this section, the combustion kinetics and mechanisms of various biofuels are evaluated.

5.1. Biodiesel Combustion

Recent studies have focused on unravelling the fundamental chemical kinetics governing biodiesel combustion, as shown below.

(a) Detailed Chemical Kinetic Models

Significant progress has been made in developing detailed chemical kinetic models for biodiesel surrogates such as methyl decanoate, methyl oleate [103]. These models, often comprising of thousands of reactions, are

crucial for accurately predicting ignition delay, flame speed, and the formation of key intermediates. They reveal that the initial breakdown of the ester moiety and the long hydrocarbon chain proceeds through hydrogen abstraction, leading to the formation of alkyl and ester radicals.

(b) Low-Temperature Combustion (LTC) Chemistry

The presence of the ester group influences the low-temperature oxidation pathways. Recent studies in engines operating in LTC modes, such as Homogeneous Charge Compression Ignition, show that the two-stage ignition behavior of biodiesel is distinct [104]. The first stage is governed by the formation and decomposition of hydroperoxy-alkyperoxy species, a process influenced by the double bonds in unsaturated FAMEs. This understanding is vital for controlling ignition timing and reducing NO_x and soot formation in advanced combustion strategies.

(c) Soot Formation and Oxidation

While biodiesel's oxygen content generally reduces soot emissions by promoting the oxidation of soot precursors (like polycyclic aromatic hydrocarbons, PAHs) and soot particles themselves, recent findings show that the type of FAME plays a critical role [105]. Unsaturated FAMEs such as methyl oleate and methyl linoleate may have a higher tendency to form soot precursors because of the presence of C=C double bonds, which can serve as sites for radical addition and subsequent cyclization reactions. Nevertheless, the embedded oxygen still tends to lead to lower overall soot production compared to diesel.

(d) NO_x Formation Mechanisms

The long-standing issue of slightly increased Nitrogen Oxide (NO_x) emissions with biodiesel remains a focus. Recent insights confirm that the higher cetane number and the presence of oxygen in biodiesel can cause a shorter ignition delay and more advanced combustion timing, leading to higher peak cylinder temperatures, which promote the thermal Zeldovich mechanism for NO_x formation [106]. Some studies also suggest that the prompt NO_x mechanism, involving the reaction of hydrocarbon radicals with atmospheric nitrogen, might be affected by the specific radical pool generated during biodiesel combustion.

5.2 Bioethanol Combustion

Although bioethanol has been widely used and studied, recent studies have provided new insights into bioethanol combustion focusing on the following aspects:

(a) Laminar Flame Speed and Blending Effects

The laminar flame speed of bioethanol exceeds that of gasoline, which can result in faster combustion and better thermal efficiency. Recent research on bioethanol-gasoline blends has shown a non-linear pattern in flame speed as ethanol content increases [107]. This is due to the complex chemical interactions between ethanol and the various hydrocarbon components of gasoline, impacting the overall radical pool and heat release rate.

(b) Aldehyde Emissions in Advanced Engines

A significant new insight concerns the formation of aldehydes, particularly formaldehyde and acetaldehyde, during bioethanol combustion, especially in advanced engines like Gasoline Direct Injection (GDI) and HCCI engines [108]. While bioethanol combustion produces fewer PAHs and soot than gasoline, the partial oxidation of ethanol can lead to higher concentrations of these toxic aldehydes. Research is now focused on understanding the kinetic pathways leading to their formation and developing strategies to mitigate them, such as optimizing injection strategies and combustion chamber design.

(c) Cool Flame and Negative Temperature Coefficient (NTC)

Bioethanol exhibits a less pronounced NTC behaviour compared to gasoline, meaning its ignition delay does not increase as significantly with temperature in the intermediate temperature range [109]. This has implications for engine knock and the operational window of HCCI engines. Understanding the specific reactions that govern this behaviour is crucial for developing accurate predictive models for engine control.

(d) Impact on Particulate Matter

While ethanol is generally considered to reduce particulate matter (PM) emissions, recent studies using sensitive measurement techniques have shown that even low-level ethanol blends can influence the size, number, and composition of nanoparticles emitted [110]. The formation of these ultrafine particles is an area of active investigation, with implications for human health and air quality.

5.3 Biogas Combustion

Biogas, primarily a mixture of methane (CH_4) and carbon dioxide (CO_2), presents unique combustion challenges due to the high dilution and lower energy density compared to natural gas. Emerging research is focused on improving its combustion stability, efficiency, and understanding its unique chemical kinetics.

(a) Chemical Kinetic Modelling of Diluted Flames

The high CO_2 content in biogas acts as a diluent, significantly affecting the flame speed, flammability limits, and heat release rate. Emerging research involves the development and validation of detailed chemical kinetic models that accurately account for the third-body effects of CO_2 on key reactions in the methane oxidation pathway [111]. These models are essential for designing efficient biogas combustors and engines.

(b) Combustion Instabilities and Lean Blowout

Biogas flames are more susceptible to instabilities and lean blowout, especially in gas turbines and industrial burners. Current research is investigating the coupling between fluid dynamics, acoustics, and chemical kinetics that drives these instabilities [112]. Understanding the chemical kinetic response of biogas flames to pressure and velocity fluctuations is crucial for developing robust and reliable combustion systems.

(c) Hydrogen Enrichment

A significant area of emerging research is the enrichment of biogas with hydrogen (H_2). Even small amounts of hydrogen can drastically improve the combustion characteristics of biogas [113], including increasing the flame speed, extending the lean flammability limit, and enhancing flame stability. Researchers are actively studying the chemical kinetic interactions between the CH_4, CO_2, and H_2 to optimize the blending strategy and maximize the benefits. [114] reported that enrichment of methane with hydrogen on a mass basis up to 6% reduces CO emission considerably and increases NO_x emission moderately.

(d) Pollutant Formation in Diluted Flames

The presence of CO_2 and the typically lower combustion temperatures in biogas flames influence pollutant formation. While NO_x emissions are generally lower due to reduced peak temperatures, the formation of carbon monoxide (CO) can be a concern, especially under lean conditions. Research is focused on understanding the CO burnout reactions in the presence of high CO_2 concentrations and developing strategies for complete combustion [115].

5.4. Combustion of Other Advanced Biofuels

Advanced biofuels, such as bio-oils produced from the fast pyrolysis of biomass, represent a promising but challenging frontier in renewable energy. These fuels are complex mixtures of hundreds of organic compounds, including water, acids, aldehydes, ketones, furans, and phenols, which makes their combustion chemistry incredibly intricate. Recent studies have focused on the following aspects:

(a) Combustion of Individual Components

Researchers have studied detailed kinetic models for compounds like levoglucosan (a sugar derivative), furfural, and various phenolic compounds [116]. This bottom-up approach helps to identify the key reaction pathways and intermediate species that are important in the overall combustion process.

(b) Challenges of High Water and Oxygen Content

Bio-oils typically contain a significant amount of water (15–30%) and oxygen (35–40%). This high water content can lead to ignition difficulties and lower flame temperatures [117]. The high oxygen content, while potentially beneficial for reducing soot, is present in various functional groups (hydroxyl, carboxyl, etc.), each with a different impact on the combustion chemistry. Research is focused on understanding how these oxygenated species break down and interact during combustion [118].

(c) Droplet Combustion and Micro-explosions

The multicomponent nature of bio-oil leads to interesting droplet combustion phenomena. As a bio-oil droplet heats up, the more volatile components vaporize first, which can lead to a build-up of pressure inside the droplet and subsequent ‘micro-explosions [119]. These events enhance fuel-air mixing and combustion efficiency but also pose challenges for predictable and controlled combustion.

(d) Catalytic Combustion and Upgrading

Due to the challenges of direct combustion, significant research is being directed towards the catalytic upgrading of bio-oils to improve their properties before combustion [120]. Furthermore, catalytic combustion, where a catalyst is used to facilitate the oxidation of the fuel at lower temperatures, is being explored to burn low-

quality bio-oils and pyrolysis products more efficiently and with fewer pollutants. This includes investigating catalysts that are resistant to coking and poisoning from the complex components of bio-oils [121].

6. Challenges and Future Directions

Combustion of biofuels face challenges arising from varying chemical and physical properties compared to fossil fuels. This variation results in complexities such as lower energy yields and increased emissions. Future directions involve developing advanced biofuels from non-food sources, improving combustion technologies for higher efficiency and lower emissions, and optimizing biofuel production processes for sustainability. Figure 2 shows a link in the recent advances, current challenges and the future directions in biofuel combustion chemistry.

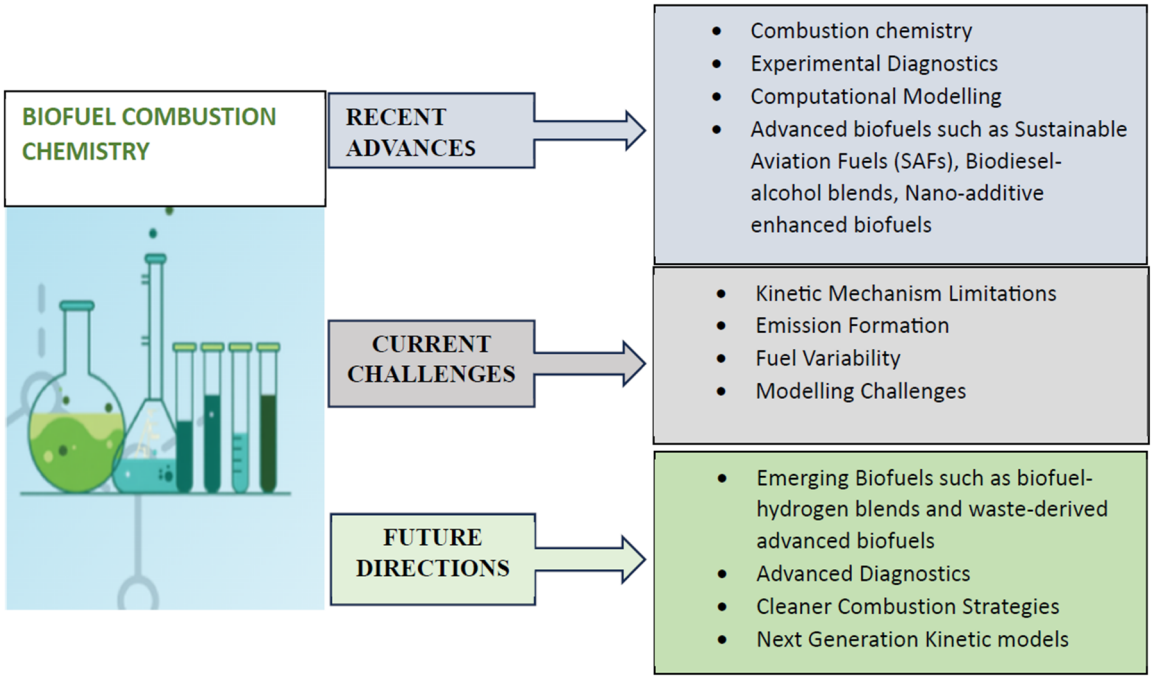

Figure 2. Recent advances, current challenges and future directions.

6.1. Emissions Reduction Strategies

One of the main challenges in biofuel combustion is the control of emissions of NO_x, CO and particulates and unburnt hydrocarbons. Generally, biofuels emit less harmful by-products compared to conventional fuels. However, due to their incomplete combustion, biofuels such as biodiesel show higher NO_x emissions, which could become a serious concern if their usage becomes more widespread [122]. Emissions from biofuel (biodiesel and bioethanol blends) combustion can be significantly mitigated by implementing low-temperature combustion (LTC) strategies such as PCCI (Premixed Charge Compression Ignition), HCCI (Homogeneous Charge Compression Ignition) and RCCI (Reactivity-Controlled Compression Ignition). These advanced methods lower peak combustion temperatures, which in turn substantially reduce nitrogen oxides (NO_x) and particulate matter (PM) emissions often by about 90% [123]. By better mixing fuel and air and carefully controlling ignition timing (especially in RCCI), these systems ensure cleaner combustion process. While they may require additional oxidation catalysts to handle elevated levels of CO and unburned hydrocarbons, they offer a promising route to cleaner internal combustion engines when used with biofuels.

A study evaluated a low-cost emission reduction system for biogas combustion, which included a chemical scrubber and thermophilic biofilter, as an alternative to traditional oxidative catalysts. The research proved that the chemical scrubber moderately decreased emissions of NO_x (28–39%), CO (19–31%), and VOCs (22–24%). The scrubber eliminated over 95% of formaldehyde when air and hydrogen peroxide were added. While the biofilter had a minor impact on VOC and odour reduction, the combined system enabled biogas engines to function at high efficiency while staying within emission limits for most of the regulated substances [124]. Emission problems associated with the direct use of biodiesel in internal combustion engines can be mitigated by making blends with biodiesel using diesel fuel in different ratios and incorporating fuel additives [125]. The emission characteristics of biofuels are provided in Table 5.

Table 5. Emission characteristics of biofuels.

Emission	Bioethanol	Biodiesel	Biogas	Reference
CO	20–40% reduction compared to neat gasoline	10–30% reduction compared to pure diesel	Very low (efficient oxidation)	[126]
CO_2	Slightly lower per MJ than gasoline	Slightly higher than diesel (but lower lifecycle)	High at combustion point but low lifecycle emissions	[127]
NO_x	Neutral to slight decrease (0–10%)	10–30% reduction	Variable: low to moderate depending on CH_4/CO_2 ratio (28–39%) emission reduction using a low-cost scrubber	[124,128]
PM (soot)	(40–50%) reduction compared to diesel	(20–60%) reduction	Near-zero soot formation	[129]
HC (unburned hydrocarbons)	Moderate reduction	19.3% reduction	Methane slip possible (CH_4 emissions)	[130]
SO_x	Almost zero	90% emission reduction	Very low	[131]

6.2. Improving Combustion Efficiency and Stability

Biodiesel degrades over time due to the presence of unsaturated fatty acid methyl esters (FAMEs), oxygen, heat, and trace metals. Antioxidants are a proven and widely used method to delay or prevent this degradation. The oxidative stability of biodiesel can be improved with antioxidants that interrupt free radical chain reactions. As highlighted by [132], synthetic antioxidants like butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), and tert-butyl hydroquinone (TBHQ) are effective but may raise cost and toxicity concerns. Natural antioxidants, such as flavonoids and phenolics from plant extracts, provide eco-friendly alternatives with strong antioxidative properties and better solubility. Their effectiveness depends on factors like concentration and chemical structure, although excessive amounts can act as pro-oxidants. Synergistic blends and emerging nanotechnology-based antioxidants also show promise for enhancing biodiesel stability.

Biodiesel combustion efficiency can be improved by optimizing blend ratios such as B10 or B20, which enhance combustion by balancing viscosity, density, and oxygen content. The naturally higher cetane number and oxygen content of biodiesel promote shorter ignition delay and more complete combustion. Although biodiesel has a lower calorific value than diesel, its combustion efficiency improves under higher engine loads and temperatures. Engine tuning such as adjusting injection timing and pressure also plays a critical role in maximizing thermal efficiency and reducing fuel consumption [106]. Biogas has low calorific value and high CO_2 content which presents significant challenges in maintaining stable combustion, particularly in excess air conditions. These issues can be solved by upgrading biogas to remove CO_2 and H_2S, controlling the air-fuel ratio, using turbocharging to improve intake conditions, and employing pilot diesel injections or advanced ignition systems to ensure reliable ignition. Engine design modifications across all three fuels such as optimizing combustion chamber geometry and swirl also play a vital role in enhancing turbulence, mixing, and flame propagation, ultimately leading to more efficient and stable

6.3. Expanding the Range of Viable Biofuels

Biofuels such as ethanol and biodiesel derived from food crops have raised concerns over food security and land use. Therefore, research is currently geared towards exploring a wider variety of non-food and waste derived feedstocks. These include lignocellulosic biomass such as crop residues, agricultural and forest residues, algae, municipal solid waste, and carbon-rich gases like CO and CO_2, which can be converted into fuels using thermochemical, biochemical or catalytic processes. Apart from feedstock diversification, there is a growing interest in producing advanced biofuels with enhanced combustion characteristics and energy density. These include furan-based compounds for high-performance applications [133]; oxygenated fuels like dimethyl ether (DME) that offer soot-free combustion [134] and butanol which has a higher energy content and better compatibility with petrol engines that that of ethanol [135].

Integrating biofuel production with the generation of high value bioproducts like bioplastics or specialty chemicals improves the economic sustainability of biorefineries and enhance holistic utilization of feedstocks. Together, these strategies are paving the way for a more diverse and resilient biofuel landscape that supports carbon neutrality and clean energy access [136]. Finally, hybrid conversion methods that combine biological and thermochemical processing enable the efficient transformation of complex structured biomass into a broader spectrum of fuels, including aviation biofuels and other alternatives that can replace petroleum-derived fuels. These fuels can be tailored to enhance engine performance, cut emissions, and serve specific sectors, such as in shipping, aviation, or heavy-duty transport.

6.4. Research Needs and Opportunities

The field of biofuel combustion chemistry is increasingly becoming pivotal as global efforts are directed towards seeking cleaner and more sustainable energy alternatives. One major challenge in this area is the development of detailed and validated chemical kinetic mechanisms for a broader variety of biofuels. These include the common options like biodiesel, bioethanol, and biogas, as well as emerging fuels such as furan-based and algae-derived biofuels. Majority of these fuels contain oxygenated molecular structures with complex and less understood reaction pathways, particularly under real engine conditions involving high pressures and variable temperatures.

Accurate modelling and prediction of combustion behavior relies on high-quality experimental data. Advanced diagnostic tools such as laser-based imaging, shock tube experiments and Raman scattering play a critical role in capturing complex processes and intermediate species that define combustion chemistry. These data are important in refining kinetic models and improving their predictive capabilities. Additionally, the oxygen content and molecular structure of biofuels largely determine pollutant formation, which is a key concern, particularly emissions of nitrogen oxides (NO_x), aldehydes and particulate matter. Understanding and mitigating these emissions is essential to ensure that biofuels deliver genuine environmental benefits. Research into catalytic combustion and the use of additives such as nanoparticles or metal-based compounds offers promising pathways to enhance combustion efficiency and reduce harmful byproducts.

Another critical area of research is the performance behavior of biofuels in advanced low-temperature combustion modes, such as Homogeneous Charge Compression Ignition (HCCI) and Reactivity Controlled Compression Ignition (RCCI). These modes offer the potential for high combustion efficiencies and lower emissions but require a deeper understanding of autoignition chemistry and the formation of intermediate species [137]. More research, experimental and modeling studies are needed to address the limitations of these combustion modes [138]. Emerging opportunities in the field include the application of artificial intelligence to optimize chemical reaction mechanisms and identify reaction pathways. Investigating fuel blends and multi-fuel strategies also offer potential for improving engine performance and operational flexibility. Ultimately, achieving meaningful progress in biofuel combustion chemistry will depend on a multidisciplinary effort, combining fundamental research, computational modelling and experimental innovation, a modeling to accelerate the transition toward a cleaner energy future.

7. Conclusions

The combustion chemistry of biofuels, particularly biodiesel, bioethanol, and biogas has undergone significant advances in recent years, because of the global transition toward clean and sustainable energy resources. This review has explored the fundamental mechanisms of biofuel combustion and compared them with conventional fossil fuels. The chemical properties and performance characteristics of each biofuel type have been highlighted. Recent advances in experimental diagnostics, such as advanced spectroscopy and flame characterization, along with microkinetic studies, have substantially enhanced observation and quantification of combustion processes. Computational modeling, including factors affecting kinetic modeling, quantum chemical calculations, and emerging machine learning techniques, has expanded our predictive capabilities, enabling improved insight into complex reaction mechanisms and pollutant formation pathways. Comparative analysis of the diagnostic techniques has been done. Bioethanol, biodiesel, and biogas each offer distinct advantages and challenges in terms of ignition properties, flame stability, and emissions. Despite offering promising results (high combustion efficiency and lower emissions), particularly in low-temperature combustion regimes and fuel blending strategies, significant challenges remain. These include minimizing NO_x and soot production, improving combustion stability under variable conditions, and extending the range of viable, sustainable biofuel feedstocks. Progressive approaches, such as catalyst-aided combustion, rational fuel design based on structure-performance relationships, provide interesting opportunities for future research. The study envisions that future work involving a multidisciplinary approach that combines experimental research, computational modeling, and applied engineering will be significant to overcoming the remaining hurdles and realizing the full potential of biofuels in a decarbonized energy landscape.

Author Contributions

D.C.S.: data curation, methodology, writing—original draft; C.A.M.: conceptualization, formal analysis, supervision, writing—review and editing; M.N.C.: visualization, validation, investigation, writing—review and editing. All authors have read and agreed to the published version of the manuscript.

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The authors declare no conflict of interest.

Use of AI and AI-Assisted Technologies

No AI tools were utilized for this paper.

References

1. Islam, S.; Ghosh, S.; Su, W. Transition from Fossil Fuels to Renewables: A Comparative Analysis Between Energy-Rich and Energy-Poor Economies. *Commodities* **2026**, *5*, 9. https://doi.org/10.3390/commodities5020009.
2. As'ad, S. Why Renewable Energy Gained Attention and Demand Globally? *Nat. Environ. Pollut. Technol.* **2024**, *23*, 467–473. https://doi.org/10.46488/NEPT.2024.v23i01.042.
3. IPCC. Climate Change 2022—Mitigation of Climate Change—Full Report, 2022. Available online: https://www.ipcc.ch/report/ar6/wg3/ (accessed on 6 June 2025).
4. IEA. Africa Energy Outlook 2022: World Energy Outlook Special Report (Revised in 2023). Available online: https://www.iea.org/reports/africa-energy-outlook-2022 (accessed on 6 June 2025).
5. Chang, J.H.; Selvaraj, S.; Manikandan, S.; et al. A Comprehensive Review of Biomass Utilization for Sustainable Biofuel and Biocomponent Development. *Biomass Bioenergy* **2025**, *202*, 108167. https://doi.org/10.1016/j.biombioe.2025.108167.
6. Torres Nazari, M.; Mazutti, J.; Caroline Girardi Basso, L.; et al. Biofuels and Their Connections with the Sustainable Development Goals: A Bibliometric and Systematic Review. *Environ. Dev. Sustain.* **2021**, *23*, 11139–11156. https://doi.org/10.1007/s10668-020-01110-4.
7. Kang, H.; Li, G.; Gao, J. Development of Bio-Diesel to Achieve Sustainable Development Goal 7. *Front. Energy Res.* **2023**, *10*, 1057336. https://doi.org/10.3389/fenrg.2022.1057336.
8. Raman, R.; Sreenivasan, A.; Kulkarni, N.V.; et al. Analyzing the Contributions of Biofuels, Biomass, and Bioenergy to Sustainable Development Goals. *iScience* **2025**, *28*, 112157. https://doi.org/10.1016/j.isci.2025.112157.
9. Sarma, H.H.; Paul, A.; Sonowal, S.; et al. Transition, Carbon Neutrality and Green Economy. **2024**, *24*, 92–98. https://doi.org/10.51470/PLANTARCHIVES.2024.v24.no.2.012.
10. Yılbaşı, Z. Biofuels, E-Fuels, and Waste-Derived Fuels: Advances, Challenges, and Future Directions. *Sustainability* **2025**, *17*, 6145. https://doi.org/10.3390/su17136145.
11. Nasreen, S.; Nasreen, S.; Parveen, K.; et al. Biofuels as Emerging and Sustainable Alternatives to Fossil Fuels: Environmental, Energetic, and Economic Perspectives. In *Recent Trends in Lignocellulosic Biofuels and Bioenergy*; Springer: Singapore, 2025; pp. 1–21. https://doi.org/10.1007/978-981-96-4636-4_1.
12. Aggarwal, N.; Kumar, N.; Mittal, M. Opportunities and Challenges for Use of Bioethanol as Transport Fuel: A Global Perspective. In *Biofuels and Bioenergy*; Springer: Cham, Switzerland, 2022; pp. 191–199. https://doi.org/10.1007/978-3-031-05091-6_15.
13. Kasturappa, G.; Bhavya, N.; Rangaiah, K.M. Biofuels: The Vital Source of Renewable Energy. In *Recent Advances in Agricultural Sciences and Technology*; Dilpreet Publishing House Ariana Publishers & Distributors New Delhi: Delhi, India, 2023.
14. Kabeyi, M.J.B.; Olanrewaju, O.A. Relationship between Electricity Consumption and Economic Development. In Proceedings of the International Conference on Electrical, Computer and Energy Technologies (ICECET 2021), Cape Town, South Africa, 9–10 December 2021. https://doi.org/10.1109/ICECET52533.2021.9698413.

15. Ali, N.A.; Shakor, Z.M.; Al-Zuhairi, F.K.; et al. Thermochemical and Biochemical Routes for Sustainable Biofuel Production: A Review. *Sustain. Chem. Environ.* **2026**, *13*, 100321. https://doi.org/10.1016/j.scenv.2026.100321.
16. Liu, X.; Law, C.K.; Yang, B. Recent Research Progress in Combustion Kinetics of Biomass-Derived Oxygenated Fuels. *Engineering* **2025**, *59*, 60–81. https://doi.org/10.1016/j.eng.2025.10.012.
17. Malik, K.; Capareda, S.C.; Kamboj, B.R.; et al. Biofuels Production: A Review on Sustainable Alternatives to Traditional Fuels and Energy Sources. *Fuels* **2024**, *5*, 157–175. https://doi.org/10.3390/fuels5020010.
18. Broda, M.; Yelle, D.J.; Serwańska, K. Bioethanol Production from Lignocellulosic Biomass—Challenges and Solutions. *Molecules* **2022**, *27*, 8717.
19. Novia, N.; Melwita, E.; Jannah, A.M.; et al. Current Advances in Bioethanol Synthesis from Lignocellulosic Biomass: Sustainable Methods, Technological Developments, and Challenges. *J. Umm Al-Qura Univ. Appl. Sci.* **2025**. https://doi.org/10.1007/s43994-025-00212-x.
20. Saha, N.; Smith, R.C.; Klinger, J. Opportunities and Challenges in Thermochemical Conversion of Municipal Solid Waste: A Comprehensive Review. *Fuel Process. Technol.* **2026**, *286*, 108447. https://doi.org/10.1016/j.fuproc.2026.108447.
21. Suhara, A.; Karyadi Herawan, S.G.; et al. Biodiesel Sustainability: Review of Progress and Challenges of Biodiesel as Sustainable Biofuel. *Clean Technol.* **2024**, *6*, 886–906. https://doi.org/10.3390/cleantechnol6030045.
22. Elgharbawy, A.S.; Sadik, W.A.; Sadek, O.M.; et al. A Review on Biodiesel Feedstocks and Production Technologies. *J. Chil. Chem. Soc.* **2021**, *65*, 5098–5109. https://doi.org/10.4067/S0717-97072021000105098.
23. Mayekar, J. Comparative Study of Biofuels and Conventional Fuels. In *Advances of nanoparticles in Energy and Environment Technologies*; Mahi Publication: Gujarat, India, 2024; pp. 60–76.
24. IEA. *Outlook for Biogas and Biomethane: Prospects for Organic Growth*; OECD Publishing: Paris, France, 2020. https://doi.org/10.1787/040c8cd2-en.
25. Abdulnaim, A.M.; Elkholy, A.H.; Elmously, M.; et al. On the Flame Structure and Emission Characteristics of Biogas Combustion Using the Double Flame Co-Firing Concept. *Energy* **2025**, *335*, 138312. https://doi.org/10.1016/j.energy.2025.138312.
26. Yang, S.; Jia, M. A Bio-Diesel Chemical Kinetic Mechanism Based on Decoupling Methodology and Detailed $H_2/O_2/CO/C_1$~C_3 Mechanism. *Front. Mech. Eng.* **2019**, *5*. https://doi.org/10.3389/fmech.2019.00021.
27. Boichenko, S.; Yakovlieva, A.; Zubenko, S.; et al. Physical, Chemical, and Performance Properties of Biodiesel Fuels: A Comparative Study of Lipid-Based Feedstocks. *Energies* **2025**, *18*, 4274. https://doi.org/10.3390/en18164274.
28. Imwinkelried, G.; Spinosa, M.; Nacuse, J.; et al. Diesel Engine Performance and Emissions Analysis with Four Different Combinations of Diesel-Soybean Biodiesel Blends. *J. Clean. Prod.* **2025**, *492*, 144806. https://doi.org/10.1016/j.jclepro.2025.144806.
29. Dahman, Y.; Syed, K.; Begum, S.; et al. Biofuels: Their Characteristics and Analysis. In *Biopolymer-Based Materials and Bioenergy*; Woodhead Publishing: Cambridge, UK, 2019; pp. 277–325. https://doi.org/10.1016/B978-0-08-102426-3.00014-X.
30. Jameel, M.K.; Mustafa, M.A.; Ahmed, H.S.; et al. Biogas: Production, Properties, Applications, Economic and Challenges: A Review. *Results Chem.* **2024**, *7*, 101549. https://doi.org/10.1016/j.rechem.2024.101549.
31. Muntaha, N.; Rain, M.I.; Goni, L.K.M.O.; et al. A Review on Carbon Dioxide Minimization in Biogas Upgradation Technology by Chemical Absorption Processes. *ACS Omega* **2022**, *7*, 33680–33698. https://doi.org/10.1021/acsomega.2c03514.
32. Wang, N.; Wang, H.; Wang, X.; et al. Impact of CO_2 Dilution on Biogas Combustion in a Double-Layer Porous Media Burner: From Ignition to Stable Combustion. *Fuel* **2026**, *406*, 137172. https://doi.org/10.1016/j.fuel.2025.137172.
33. Barasa Kabeyi, M.J. Biogas Treatment and Upgrading Techniques. In Proceedings of the 4th Asia Pacific International Conference on Industrial Engineering and Operations Management, Ho Chi Minh City, Vietnam, 12–14 September 2023. https://doi.org/10.46254/ap04.20230266.
34. Muhaji; Sutjahjo, D.H. The Characteristics of Bioethanol Fuel Made of Vegetable Raw Materials. *IOP Conf. Ser. Mater. Sci. Eng.* **2018**, *296*, 012019. https://doi.org/10.1088/1757-899X/296/1/012019.
35. Forsberg, C.W.; Dale, B.E.; Jones, D.S.; et al. Replacing Liquid Fossil Fuels and Hydrocarbon Chemical Feedstocks with Liquid Biofuels from Large-Scale Nuclear Biorefineries. *Appl. Energy* **2021**, *298*, 117225. https://doi.org/10.1016/j.apenergy.2021.117225.
36. Elkelawy, M.; Alm-Eldin Bastawissi, H.; El Shenawy, E.A.; et al. Study of Performance, Combustion, and Emissions Parameters of DI-Diesel Engine Fueled with Algae Biodiesel/Diesel/n-Pentane Blends. *Energy Convers. Manag. X* **2021**, *10*, 100058. https://doi.org/10.1016/j.ecmx.2020.100058.
37. Malode, S.J.; Prabhu, K.K.; Mascarenhas, R.J.; et al. Recent Advances and Viability in Biofuel Production. *Energy Convers. Manag. X* **2021**, *10*, 100070. https://doi.org/10.1016/j.ecmx.2020.100070.
38. Kiteto, M.K.; Vidija, B.M.; Mecha, C.A. Production of Bioethanol from Citrus Peel Waste: A Techno-Economic Feasibility Study. *Energy Convers. Manag. X* **2025**, *26*, 100916. https://doi.org/10.1016/j.ecmx.2025.100916.

39. Xiong, Q.; Duan, Y.; Liang, D.; et al. Biofuels and Their Blends—A Review of the Effect of Low Carbon Fuels on Engine Performance. *Sustainability* **2024**, *16*, 10300. https://doi.org/10.3390/su162310300.
40. Shahi, Z.; Khajeh Mehrizi, M. Biofuel Production Technologies, Comparing the Biofuels and Fossil Fuels. In *Bioenergy Research: Revisiting Latest Development*; Springer: Singapore, 2021; pp. 1–27. https://doi.org/10.1007/978-981-33-4615-4_1.
41. Westbrook, C.K.; Naik, C.V.; Herbinet, O.; et al. Detailed Chemical Kinetic Reaction Mechanisms for Soy and Rapeseed Biodiesel Fuels. *Combust. Flam* **2011**, *158*, 742–755.
42. Parveg, A.S.M.S.; Ratner, A. Droplet-Scale Combustion Analysis of Third-Generation Biodiesel–Diesel Blends. *Energies* **2025**, *18*, 1692.
43. Pichler, C.; Nilsson, E.J.K. Pathway Analysis of Skeletal Kinetic Mechanisms for Small Alcohol Fuels at Engine Conditions. *Fuel* **2020**, *275*, 117956. https://doi.org/10.1016/j.fuel.2020.117956.
44. Kim, H.Y.; Ge, J.C.; Choi, N.J. Effects of Ethanol-Diesel on the Combustion and Emissions from a Diesel Engine at a Low Idle Speed. *Appl. Sci.* **2020**, *10*, 4153. https://doi.org/10.3390/APP10124153.
45. El-Faroug, M.O.; Yan, F.; Luo, M.; et al. Spark Ignition Engine Combustion, Performance and Emission Products from Hydrous Ethanol and Its Blends with Gasoline. *Energies* **2016**, *9*, 984. https://doi.org/10.3390/en9120984.
46. Mekonen, E.A.; Mekonnen, Y.T.; Fatoba, S.O. Thermodynamic Prediction of Biogas Production and Combustion: The Spontaneity and Energy Conversion Efficiency from Photosynthesis to Combustion. *Sci. Afr.* **2023**, *21*, e01776. https://doi.org/10.1016/j.sciaf.2023.e01776.
47. Fajobi, M.O.; Lasode, O.A.; Adeleke, A.A.; et al. Prediction of Biogas Yield from Codigestion of Lignocellulosic Biomass Using Adaptive Neuro-Fuzzy Inference System (ANFIS) Model. *J. Eng.* **2023**, *2023*, 9335814. https://doi.org/10.1155/2023/9335814.
48. Chen, W.; Huang, Z.; Chua, K.J. Sustainable Energy Recovery from Thermal Processes: A Review. *Energy Sustain. Soc.* **2022**, *12*, 46. https://doi.org/10.1186/s13705-022-00372-2.
49. Wako, F.M.; Pio, G.; Salzano, E. Laminar Burning Velocity and Ignition Delay Time of Oxygenated Biofuel. *Energies* **2021**, *14*, 3562. https://doi.org/10.3390/en14123562.
50. Giurcan, V.; Movileanu, C.; Musuc, A.M.; et al. Laminar Burning Velocity of Biogas-Containing Mixtures. A Literature Review. *Processes* **2021**, *9*, 996. https://doi.org/10.3390/pr9060996.
51. Hoang, L.V.; Nguyen, D.C.; Truong, T.H.; et al. Laminar Flame Characteristics of 2,5-Dimethylfuran (DMF) Biofuel: A Comparative Review with Ethanol and Gasoline. *Int. J. Renew. Energy Dev.* **2022**, *11*, 237–254. https://doi.org/10.14710/ijred.2022.42611.
52. Xi, S.; Wang, T.; Zhong, L.; et al. Theoretical Study on the Low-Temperature Reaction of β-Hydroxyethyl Radical and Its Optimization and Validation for Combustion Models. *Case Stud. Therm. Eng.* **2026**, *82*, 108076. https://doi.org/10.1016/j.csite.2026.108076.
53. Han, J.; Somers, L.M.T. Low-Temperature Combustion Analysis of Butanol Isomer/Diesel Blends under Reduced Oxygen Conditions in a Constant Volume Combustion Chamber. *Case Stud. Therm. Eng.* **2025**, *68*, 105929. https://doi.org/10.1016/j.csite.2025.105929.
54. Pham, P.; Pham, N.; Pham, T.; et al. Ignition Delays of Biodiesel-Diesel Blends: Investigations into the Role of Physical and Chemical Processes. *Fuel* **2021**, *303*, 121251. https://doi.org/10.1016/j.fuel.2021.121251.
55. Long, B.; Xia, Y.; Truhlar, D.G. Quantitative Kinetics of HO_2 Reactions with Aldehydes in the Atmosphere: High-Order Dynamic Correlation, Anharmonicity, and Falloff Effects Are All Important. *J. Am. Chem. Soc.* **2022**, *144*, 19910–19920. https://doi.org/10.1021/jacs.2c07994.
56. Morad, M.H. Current Status and Future Perspectives of Efficient Catalytic Conversion of Bioethanol to Value-Added Chemicals and Fuels. *Arab. J. Chem.* **2023**, *17*, 105560. https://doi.org/10.1016/j.arabjc.2023.105560.
57. Abdulnaim, A.M.; Elkholy, A.H.; Elmously, M.; et al. Analysis of Non-Reacting and Reacting Flows in Biogas/Methane Cofiring within a Double-Swirl Burner: Role of the Inner Swirler. *Exp. Therm. Fluid Sci.* **2026**, *172*, 111654. https://doi.org/10.1016/j.expthermflusci.2025.111654.
58. Mohamed, S.Y.; Kim, Y.; Fioroni, G.; et al. High-Pressure Rate Rules for Ether Alkylperoxy Radical Isomerization. *J. Phys. Chem. A* **2024**, *128*, 8220–8231. https://doi.org/10.1021/acs.jpca.4c04840.
59. Pathak, V.; Panigrahy, S. Chemical Kinetic Modeling to Study the Ignition and Oxidation of E-Fuels. In *Sustainable, Scalable and Storable E-Fuels for Decarbonising Transport Sector*; Springer: Singapore, 2025; pp. 5–25. https://doi.org/10.1007/978-981-96-7388-9_2.
60. Atmanli, A.; Yilmaz, N.; Vigil, F.M. Effect of Alcohol-Enhanced Diesel and Biodiesel Blends on Polycyclic Aromatic Hydrocarbons and Toxicity. *Energies* **2026**, *19*, 2644.
61. Sadeq, A.M.; Homod, R.Z.; Hasan, H.A.; et al. Advancements in Combustion Technologies: A Review of Innovations, Methodologies, and Practical Applications. *Energy Convers. Manag. X* **2025**, *26*, 100964. https://doi.org/10.1016/j.ecmx.2025.100964.

62. Gazeli, K.; Lombardi, G.; Aubert, X.; et al. Progresses on the Use of Two-Photon Absorption Laser Induced Fluorescence (TALIF) Diagnostics for Measuring Absolute Atomic Densities in Plasmas and Flames. *Plasma* **2021**, *4*, 145–171. https://doi.org/10.3390/plasma4010009.
63. Koegl, M.; Mull, C.; Mishra, Y.N.; et al. Characterization of Fuel/Water Mixtures and Emulsions with Ethanol Using Laser-Induced Fluorescence. *Appl. Opt.* **2020**, *59*, 1136. https://doi.org/10.1364/ao.380392.
64. Hay, M.; Parajuli, P.; Kulatilaka, W.D. Simultaneous Detection of Three Chemical Species (NO, O, O_2) Using a Single Broadband Femtosecond Laser. *Proc. Combust. Inst.* **2023**, *39*, 1435–1444. https://doi.org/10.1016/j.proci.2022.08.090.
65. Li, Z.; Brackmann, C.; Bood, J.; et al. Laser Diagnostics in Combustion and Beyond Dedicated to Prof. Marcus Aldén on His 70th Birthday. *Combust. Flame* **2024**, *263*, 113403. https://doi.org/10.1016/j.combustflame.2024.113403.
66. Agilent Technologies. *The basics of UV-Vis Spectrophotometry*; Agilent Technologies, Inc.: Santa Clara, CA, USA, 2021; pp. 5980–1397. Available online: https://www.researchgate.net/institution/Agilent/post/5f91dc68f017d4430850d083 (accessed on 6 February 2026).
67. Altarawneh, M.; Ali, L. Formation of Polycyclic Aromatic Hydrocarbons (PAHs) in Thermal Systems: A Comprehensive Mechanistic Review. *Energy Fuels* **2024**, *38*, 21735–21792. https://doi.org/10.1021/acs.energyfuels.4c03513.
68. Braga, E.; Damasceno, L.; Barros de Sousa Silva, C.; et al. ^{1}H NMR and UV-Vis as Analytical Techniques to Evaluate Biodiesel Conversion and Oxidative Stability. *Fuels* **2024**, *5*, 107–122. https://doi.org/10.3390/fuels5010007.
69. Hassing, S. What Is Vibrational Raman Spectroscopy: A Vibrational or an Electronic Spectroscopic Technique or Both? *Mod. Spectrosc. Tech. Appl.* **2020**. https://doi.org/10.5772/intechopen.86838.
70. Wallocha, T.; Poth, M. Harnessing Raman Spectroscopy for Enhanced Bioprocess Monitoring: Predictive CO_2 Analysis and Robust pH Determination in Bioreactor Off-Gas Stream. *Fermentation* **2025**, *11*, 317.
71. Calogiuri, A.; Bellisario, D.; Sciurti, E.; et al. Non-Invasive Real-Time Investigation of Colorectal Cells Tight Junctions by Raman Microspectroscopy Analysis Combined with Machine Learning Algorithms for Organ-on-Chip Applications. *Front. Bioeng. Biotechnol.* **2024**, *12*, 1458404. https://doi.org/10.3389/fbioe.2024.1458404.
72. Petrov, D.V. Features of Measuring Low CO Concentrations in N_2-Containing Mixtures at Different Temperatures Using Spontaneous Raman Spectroscopy. *Appl. Spectrosc.* **2020**, *75*, 81–86. https://doi.org/10.1177/0003702820957009.
73. Workman, J. Advancements and Emerging Techniques in Mass Spectrometry: A Comprehensive Review. *LCGC Suppl.* **2024**, 22–27. Available online: https://www.chromatographyonline.com/view/advancements-and-emerging-techniques-in-mass-spectrometry-a-comprehensive-review (accessed on 7 February 2026).
74. Shen, Y.; Cui, C.; Liu, H.; et al. Recent Contributions of Photoionization Mass Spectrometry in the Study of Typical Solid Fuel Pyrolysis. *J. Fuel Chem. Technol.* **2024**, *52*, 921–944. https://doi.org/10.1016/S1872-5813(23)60411-6.
75. Korpeh, M.; Lotfollahi, A.; Moghimi, M.; et al. Combustion Optimization of Various Biomass Types to Hydrogen-Rich Syngas: Two-Stage Pyrolysis Modeling, Methane Addition Effects, and Environmental Impact Assessment. *Int. J. Hydrogen Energy* **2025**, *133*, 458–471. https://doi.org/10.1016/j.ijhydene.2025.04.490.
76. Köhler, M.; Oßwald, P.; Krueger, D.; et al. Combustion Chemistry of Fuels: Quantitative Speciation Data Obtained from an Atmospheric High-Temperature Flow Reactor with Coupled Molecular-Beam Mass Spectrometer. *J. Vis. Exp.* **2018**, *2018*, 56965. https://doi.org/10.3791/56965.
77. Davani, A.A.; Ronney, P.D. A New Jet-Stirred Reactor for Chemical Kinetics Experiments. In Proceedings of the 10th U. S. National Combustion Meeting, College Park, Maryland, 23–26 April 2017.
78. Zhang, Y.; Jeanson, M.; Mével, R.; et al. Tailored Mixture Properties for Accurate Laminar Flame Speed Measurement from Spherically Expanding Flames: Application to $H_2/O_2/N_2$/He Mixtures. *Combust. Flame* **2021**, *231*, 111487. https://doi.org/10.1016/j.combustflame.2021.111487.
79. Dai, Y.; Weng, W.; Liu, S.; et al. Research Progress of Laser Photofragmentation-Fragment Detection Techniques in Combustion Diagnostics. *Appl. Spectrosc. Rev.* **2025**, *60*, 451–510. https://doi.org/10.1080/05704928.2025.2461317.
80. Yang, Z.; Yu, X.; Peng, J.; et al. Quantitative Planar Laser-Induced Fluorescence Technology. In *Laser Technology*; IntechOpen: London, UK, 2018. https://doi.org/10.5772/intechopen.79702.
81. Wang, Y.; Jain, A.; Schweizer, C.; et al. OH, PAH, and Sooting Imaging in Piloted Liquid-Spray Flames of Diesel and Diesel Surrogate. *Combust. Flame* **2021**, *231*, 111479. https://doi.org/10.1016/j.combustflame.2021.111479.
82. Yuan, C.; Pu, J.; Fu, D.; et al. UV-Vis Spectroscopic Detection of Formaldehyde and Its Analogs: A Convenient and Sensitive Methodology. *J. Hazard. Mater.* **2022**, *438*, 129457. https://doi.org/10.1016/j.jhazmat.2022.129457.
83. Dal Moro, R.; Melison, F.; Cocola, L.; et al. Raman Spectroscopy for Monitoring NO_x and N_2O in Combustion Products. *Sensors* **2026**, *26*, 3180. https://doi.org/10.3390/s26103180.
84. He, X.; Giese, M.; Ruwe, L.; et al. A Detailed Uncertainty Analysis of EI-MBMS Data from Combustion Experiments. *Combust. Flame* **2022**, *243*, 112012. https://doi.org/10.1016/j.combustflame.2022.112012.
85. Subramaniam, K.; Wong, K.Y.; Wong, K.H.; et al. Enhancing Biodiesel Production: A Review of Microchannel Reactor Technologies. *Energies* **2024**, *17*, 1652. https://doi.org/10.3390/en17071652.

86. Almarzooq, Y.M.; Schoegl, I.; Petersen, E.L. Laminar Flame Speed Measurements of a Gasoline Surrogate and Its Mixtures with Ethanol at Elevated Pressure and Temperature. *Fuel* **2023**, *343*, 128003. https://doi.org/10.1016/j.fuel.2023.128003.
87. Hoblos, B.; Dayma, G.; Halter, F.; et al. Laminar Flame Speeds of Methanol and Ethanol at High Pressure and Temperature Conditions: An Experimental and Modeling Approach. *Fuel* **2026**, *415*, 138358. https://doi.org/10.1016/j.fuel.2026.138358.
88. Pitsch, H. The Transition to Sustainable Combustion: Hydrogen- and Carbon-Based Future Fuels and Methods for Dealing with Their Challenges. *Proc. Combust. Inst.* **2024**, *40*, 105638. https://doi.org/10.1016/j.proci.2024.105638.
89. Wilk-Jakubowski, J.L.; Pawlik, L.; Frej, D.; et al. Data-Driven Computational Methods in Fuel Combustion: A Review of Applications. *Appl. Sci.* **2025**, *15*, 7204. https://doi.org/10.3390/app15137204.
90. Dana, A.G.; Buesser, B.; Merchant, S.S.; et al. Automated Reaction Mechanism Generation Including Nitrogen as a Heteroatom. *Int. J. Chem. Kinet.* **2018**, *50*, 243–258. https://doi.org/10.1002/kin.21154.
91. Deng, S.; Wang, L.; Kim, S.; et al. Scientific Machine Learning in Combustion for Discovery, Simulation, and Control. *Proc. Combust. Inst.* **2025**, *41*, 105796. https://doi.org/10.1016/j.proci.2025.105796.
92. Dong, X. Automatic Generation of Chemical Kinetic Models for Biofuel Oxidation and Pyrolysis. Ph.D. Thesis, Massachusetts Institute of Technology, Cambridge, MA, USA, 2024.
93. Miller, J.A.; et al. Combustion Chemistry in the Twenty-First Century: Developing Theory-Informed Chemical Kinetics Models. *Prog. Energy Combust. Sci.* **2021**, *83*, 100886. https://doi.org/10.1016/j.pecs.2020.100886.
94. Zandie, M.; Ng, H.K.; Gan, S.; et al. Development of a Reduced Multi-Component Chemical Kinetic Mechanism for the Combustion Modelling of Diesel-Biodiesel-Gasoline Mixtures. *Transp. Eng.* **2022**, *7*, 100101. https://doi.org/10.1016/j.treng.2021.100101.
95. Du, F.; Ye, T.; Wu, Y.; et al. Computational Comparison of Oxidation Stability: Sulfones vs. Fluorinated Sulfones. *Chem. Phys.* **2021**, *551*, 111328. https://doi.org/10.1016/j.chemphys.2021.111328.
96. Zhu, C.; Cao, J.P.; Yang, Z.; et al. Study on Hydrodeoxygenation Mechanism of Anisole over Ni (111) by First-Principles Calculation. *Mol. Catal.* **2022**, *523*, 111402. https://doi.org/10.1016/j.mcat.2021.111402.
97. Wan, T.; Zhou, M.; Zhao, P.; et al. Challenges in the Modeling and Simulation of Turbulent Supercritical Fluid Flows and Heat Transfer. *Propuls. Energy* **2025**, *1*, 6. https://doi.org/10.1007/s44270-024-00005-3.
98. Jaravel, T. Prediction of Pollutants in Gas Turbines Using Large Eddy Simulation. Ph.D. Thesis, Université de Toulouse, Toulouse, France, 2023.
99. Wu, G.; Zhao, Y.; Du, J.; et al. Machine Learning Potential Model for Accelerating Quantum Chemistry-Driven Property Prediction and Molecular Design. *AIChE J.* **2025**, *71*, e18741. https://doi.org/10.1002/aic.18741.
100. Sikalo, N.; Hasemann, O.; Schulz, C.; et al. A Genetic Algorithm-Based Method for the Automatic Reduction of Reaction Mechanisms. *Int. J. Chem. Kinet.* **2014**, *46*, 41–59. https://doi.org/10.1002/kin.20826.
101. Samadian, D.; Muhit, I.B.; Dawood, N. Application of Data-Driven Surrogate Models in Structural Engineering: A Literature Review. *Arch. Comput. Methods Eng.* **2024**, *32*, 735–784. https://doi.org/10.1007/s11831-024-10152-0.
102. Quaye, E.K.; et al. A Review of Hybrid Computational Fluid Dynamics and Machine Learning Approaches for the Combustion of Alternative Fuels. *J. Energy Inst.* **2026**, *124*, 102384. https://doi.org/10.1016/j.joei.2025.102384.
103. Alviso, D.; Costa, M.; Heberle, L.; et al. Chemical Kinetic Mechanism for Diesel/Biodiesel/Ethanol Surrogates Using n-Decane/Methyl-Decanoate/Ethanol Blends. *J. Braz. Soc. Mech. Sci. Eng.* **2020**, *42*, 100. https://doi.org/10.1007/s40430-020-2186-9.
104. Virt, M.; Zöldy, M. Realization of Low Temperature Combustion in an Unmodified Diesel Engine. *Cogn. Sustain.* **2024**, *3*. https://doi.org/10.55343/cogsust.104.
105. Kiraithe, R.M.; Tanui, J.K.; Kioni, P.N. Influence of Major Biodiesel Components on Soot Formation in Biodiesel Co-Flow Jet Flames. *J. Sustain. Res. Eng.* **2024**, *8*, 1–16.
106. Wu, G.; Ge, J.C.; Choi, N.J. A Comprehensive Review of the Application Characteristics of Biodiesel Blends in Diesel Engines. *Appl. Sci.* **2020**, *10*, 8015. https://doi.org/10.3390/app10228015.
107. Ronan, P.; Pierre, B.; Christine, M.-R.; et al. Laminar Flame Speed of Ethanol/Ammonia Blends–An Experimental and Kinetic Study. *Fuel Commun.* **2022**, *10*, 100052. https://doi.org/10.1016/j.jfueco.2022.100052.
108. Al-Rawashdeh, H.; Hasan, A.O.; Gomaa, M.R.; et al. Determination of Carbonyls Compound, Ketones and Aldehydes Emissions from CI Diesel Engines Fueled with Pure Diesel/Diesel Methanol Blends. *Energies* **2022**, *15*, 7933. https://doi.org/10.3390/en15217933.
109. Boot, M.D.; Tian, M.; Hensen, E.J.M.; et al. Impact of Fuel Molecular Structure on Auto-Ignition Behavior—Design Rules for Future High Performance Gasolines. *Prog. Energy Combust. Sci.* **2017**, *60*, 1–25. https://doi.org/10.1016/j.pecs.2016.12.001.
110. Zhang, M.; Ge, Y.; Wang, X.; et al. Particulate Emissions from Direct-Injection and Combined-Injection Vehicles Fueled with Gasoline/Ethanol Match-Blends—Effects of Ethanol and Aromatic Compositions. *Fuel* **2021**, *302*, 121010. https://doi.org/10.1016/j.fuel.2021.121010.

111. Khan, F.; Elbaz, A.; Saxena, S.; et al. Effect of CO_2 Dilution on Methane/Air Flames at Elevated Pressures: An Experimental and Modeling Study. *Energy Fuels* **2021**, *35*, 2639–2653. https://doi.org/10.1021/acs.energyfuels.0c03568.
112. Abdulnaim, A.; Elkholy, A.; Elmously, M.; et al. On the stability and characteristics of Biogas/Methane/Air Flames fired by a Double Swirl Burner. *Flow Turbul. Combust.* **2024**, *112*, 751–767. https://doi.org/10.1007/s10494-023-00427-0.
113. Benaissa, S.; Adouane, B.; Ali, S.M.; et al. Effect of Hydrogen Addition on the Combustion Characteristics of Premixed Biogas/Hydrogen-Air Mixtures. *Int. J. Hydrogen Energy* **2021**, *46*, 18661–18677. https://doi.org/10.1016/j.ijhydene.2021.02.225.
114. Patel, V.; Shah, R. Effect of Hydrogen Enrichment on Combustion Characteristics of Methane Swirling and Non-Swirling Inverse Diffusion Flame. *Int. J. Hydrogen Energy* **2019**, *44*, 28316–28329. https://doi.org/10.1016/j.ijhydene.2019.09.076.
115. Ashini, H.; Tabejamaat, S.; Bastani, M. Experimental and Numerical Study on Combustion of Biogas/Lean-Hydrogen Syngas Mixtures in a Microturbine Combustor. *Int. J. Hydrogen Energy* **2025**, *102*, 1–19. https://doi.org/10.1016/j.ijhydene.2025.01.001.
116. Liu, Y.; Zheng, W.; Wu, Y.; et al. Study on Pyrolysis Behaviors and Characteristics, Thermodynamics, Kinetics, and Volatiles of Single-Base Propellant, a Typical Energy-Containing Material. *Fire* **2023**, *6*, 370. https://doi.org/10.3390/fire6100370.
117. Wang, Y.; Maes, N.; Cuijpers, M.; et al. Spray Combustion of Fast-Pyrolysis Bio-Oils under Engine-like Conditions. *Energy Convers. Manag. X* **2023**, *20*, 100433. https://doi.org/10.1016/j.ecmx.2023.100433.
118. Han, J.; Somers, L.M.T.; van de Beld, B. Combustion and Emission Characteristics of Hydrotreated Pyrolysis Oil on a Heavy-Duty Engine. *Fuel* **2023**, *351*, 128888. https://doi.org/10.1016/j.fuel.2023.128888.
119. Wang, J.; Zhang, Q.; Liang, K.; et al. Micro-Explosion Enhanced Combustion of Jatropha Oil/2,5-Dimethylfuran (DMF) Blended Fuel Droplets. *Fuel* **2023**, *331*, 125807. https://doi.org/10.1016/j.fuel.2022.125807.
120. Reza, M.S.; et al. Influence of Catalyst on the Yield and Quality of Bio-Oil for the Catalytic Pyrolysis of Biomass: A Comprehensive Review. *Energies* **2023**, *16*, 5547. https://doi.org/10.3390/en16145547.
121. Awodun, K.; He, Y.; Wu, C.; et al. Catalytic Pyrolysis of Bio-Waste in Synthesis of Value-Added Products: A Systematic Review. *Fuel Process. Technol.* **2025**, *275*, 108258. https://doi.org/10.1016/j.fuproc.2025.108258.
122. Jayaraj, J.J.; Mageshwaran, G.; Joseph, B.; et al. Various Strategies for Reducing NO_x Emissions of Biodiesel Fuel Used in Conventional Diesel Engines: A Review. *Chem. Eng. Commun.* **2017**, *204*, 1202–1223. https://doi.org/10.1080/00986445.2017.1353500.
123. Arda, E. HCCI, PCCI and RCCI Low Temperature Combustion Strategies: A Comparative Assessment. In *Pioneer Research in Engineering*; All Sciences Academy: Paris, France, 2025.
124. Dobslaw, D.; Engesser, K.H.; Störk, H.; et al. Low-Cost Process for Emission Abatement of Biogas Internal Combustion Engines. *J. Clean. Prod.* **2019**, *227*, 1079–1092. https://doi.org/10.1016/j.jclepro.2019.04.258.
125. Bitire, S.O.; Nwanna, E.C.; Jen, T.C. The Impact of CuO Nanoparticles as Fuel Additives in Biodiesel-Blend Fuelled Diesel Engine: A Review. *Energy Environ.* **2023**, *34*, 2259–2289. https://doi.org/10.1177/0958305X221089217.
126. Iodice, P.; Amoresano, A.; Langella, G. A Review on the Effects of Ethanol/Gasoline Fuel Blends on NO_x Emissions in Spark-Ignition Engines. *Biofuel Res. J.* **2021**, *8*, 1465–1480. https://doi.org/10.18331/brj2021.8.4.2.
127. Abdellatief, T.M.; Handawy, M.K.M., M.; Kamel, A.; et al. Fueling the Future: Emission Characteristics and Sustainability of High-Octane Gasoline Biofuels Derived from Lignocellulosic Biomass. *Results Eng.* **2025**, *26*, 105347. https://doi.org/10.1016/j.rineng.2025.105347.
128. Peng, D.X. Exhaust Emission Characteristics of Various Types of Biofuels. *Adv. Mech. Eng.* **2015**, *7*. https://doi.org/10.1177/1687814015593036.
129. Sukjit, E.; Klinkaew, N.; Pumpuang, A.; et al. Particulate Matter Characteristics and Emissions of Waste- and Bio-Derived Fuels in Diesel Engine Applications. *Clean. Eng. Technol.* **2025**, *28*, 101056. https://doi.org/10.1016/j.clet.2025.101056.
130. Lee, K.; Cho, H. Comparative Analysis of Performance and Emission Characteristics of Biodiesels from Animal Fats and Vegetable Oils as Fuel for Common Rail Engines. *Energies* **2024**, *17*, 1711. https://doi.org/10.3390/en17071711.
131. Christopher Selvam, D.; et al. The Role of Biodiesel in Marine Decarbonization: Technological Innovations and Ocean Engineering Challenges. *Results Eng.* **2025**, *25*, 103974. https://doi.org/10.1016/j.rineng.2025.103974.
132. Bello, U.; Adamu, H.; Samsuri, S.; et al. Improving Biodiesel Oxidative Stability Using Antioxidants: An Insight into the Research Trends and Future Prospects from a Bibliometric Approach. *Results Eng.* **2025**, *26*, 105185. https://doi.org/10.1016/j.rineng.2025.105185.
133. Ahmad, F.B.; Kalam, M.A.; Zhang, Z.; et al. Sustainable Production of Furan-Based Oxygenated Fuel Additives from Pentose-Rich Biomass Residues. *Energy Convers. Manag. X* **2022**, *14*, 100222. https://doi.org/10.1016/j.ecmx.2022.100222.
134. Luo, Y.; He, Y.; Liu, C.; et al. Combustion Characteristics of Biodiesel with Different Dimethyl Ether Blending Strategies. *Fuel* **2023**, *332*, 126078. https://doi.org/10.1016/j.fuel.2022.126078.
135. Liu, H.; et al. Investigation on Blending Effects of Gasoline Fuel with n-Butanol, DMF, and Ethanol on the Fuel Consumption and Harmful Emissions in a GDI Vehicle. *Energies* **2019**, *12*, 1845. https://doi.org/10.3390/en12101845.

136. Singh, N.; Ogunseitan, O.A.; Wong, M.H.; et al. Sustainable Materials Alternative to Petrochemical Plastics Pollution: A Review Analysis. *Sustain. Horiz.* **2022**, *2*, 100016. https://doi.org/10.1016/j.horiz.2022.100016.
137. Agarwal, A.K.; Singh, A.P.; García, A.; et al. Challenges and Opportunities for Application of Reactivity-Controlled Compression Ignition Combustion in Commercially Viable Transport Engines. *Prog. Energy Combust. Sci.* **2022**, *93*, 101028. https://doi.org/10.1016/j.pecs.2022.101028.
138. Nachimuthu, P.; Kumar, N.; Chinnaswamy, S.; et al. A Review on Recent Developments of Smart Cities. *AIP Conf. Proc*. **2023**, *2857*, 020017. https://doi.org/10.1063/5.0164311.