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Evaluation of Jojoba Oil Biodiesel as a Potential Fuel for Combustion Application

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Abstract

The demand for efficient energy systems is rising due to environmental issues and the decline of fossil fuels. Therefore, the studies are exploring the use of biofuels as an alternative fuel. The focus of this study is to produce biodiesel from jojoba oil and use it along with other fuels in internal combustion engines. The transesterification method was used for the production of biodiesel using methanol and a catalyst (sodium hydroxide), which yielded long-chain fatty acid methyl esters (C16–C20) and physicochemical properties were investigated. Gas chromatography-mass spectrometry and nuclear magnetic resonance were used to analyze raw jojoba oil and biodiesel. Moreover, the ignition delay (ID) time and derived cetane number (DCN) were measured by an ignition quality tester (IQT). The density (870 kg m^{-3}) and viscosity (4.21 mm^2 s^{-1}) of the biodiesel were comparable to ASTM D6751-24 requirements and were also closely aligned with US 2D petrodiesel quality. The IQT test demonstrated that biodiesel produced from jojoba oil has a higher DCN and shorter ID than US 2D petro-diesel. Thus, the overall results adequately illustrate the potential to use biodiesel as a sustainable energy application.

Keywords

jojoba oil biodiesel, alternative fuels, combustion applications, ignition properties, sustainable energy

1 Introduction

Emissions, energy security, and stringent environmental regulations are among the factors driving global interest in the use of biofuels. Bio-derived fuels include alcohols and biodiesel. Alcohols are derived mainly from starch and sugar canes while biodiesels are usually produced from vegetable oils and fats, through transesterification to yield large molecules of fatty acid alkyl esters (FAAEs). The resulting FAAEs would have properties similar to conventional diesel fuel and could be used as blends or neat fuel in the engine. Blends of biodiesel with natural diesel fuel could increase the reactivity of the diesel fuel due to its high cetane number (CN) and could even lower the emission of unburnt hydrocarbon to the atmosphere [1]. Previous literature [2–6] reported on biodiesel production from non-edible jojoba oil. The studies reported that biodiesels produced from jojoba oil consist mainly of large molecules of FAAEs in the range of C20-C24. Al-Shanableh et al. [7] converted jojoba oil extracted from Mesaoria Plain plants into biodiesel using the supercritical methanol (SCM) method in a supercritical reactor.

Jojoba oil is obtained from jojoba seed, a perennial plant mainly grown in the desert. It is extremely tolerant to different harsh environments, including hot sun, high altitude, and salty water [3]. The oil is extracted from the seed using organic solvents or by employing much cleaner methods, such as the use of supercritical fluids like CO_2 [8]. Nearly half of the seed is made of jojoba oil, which looks like liquid wax. The extracted wax mainly consists of long monounsaturated esters, which can be trans-esterified using a catalyst such as NaOH to large molar mass FAAEs and jojoba alcohol. After washing off the alcohol, the FAAEs can be used as a biodiesel fuel or further refined to produce other fuels with high octane numbers that can be used as octane boosters for gasoline fuels [2, 3].

Both spark ignition (SI) and compression ignition (CI) engines have been designed for the use of conventional

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petroleum-derived fuels. It is only recently that the use of biofuels (biodiesel and bioethanol) has been enabled on these systems through detailed combustion studies [1, 2]. These studies provide engine designers with a database of the combustion properties of each fuel. Many pieces of literature are available on the potential of first-generation biofuel sources such as the soybean [2], palm [9–12] and cooking oil [9], but little is available on jojoba oil. Jojoba-derived biofuel can be used in combustion applications; however, there is currently little progress in understanding its combustion behavior, and no systems have been designed to use this fuel. Despite its potential, few studies have attempted to understand the combustion properties of jojoba oil [4, 6, 13]. These studies measured the physical properties and emission (NO_x, CO, CO_2) of blends of crude jojoba oil with conventional diesel fuel. They found that adding the oil to conventional diesel fuel in diesel engines reduces NO_x emissions but increases CO_2 and CO emissions.

Recent studies have significantly advanced the understanding of biodiesel combustion characteristics. Recently, Zhang et al. [14] evaluated the different generations of biodiesel in diesel engines in terms of production, properties, combustion, performance, and emission characteristics. For instance, Ooi et al. [15] recently evaluated quaternary blends composed of diesel, palm-oil biodiesel, ethanol, and diethyl ether, identifying optimal blend ratios (6.78 vol% diethyl ether and 20.00 vol% ethanol to achieve improved engine performance and reduced emissions in light-duty diesel engines. Ooi et al. [16] studied droplet combustion in diesel palm biodiesel blends, which revealed distinct combustion behaviors. They found a 56.3% improvement in the burning rate for palm biodiesel droplets. Chow et al. [17] investigated the role of ethanol addition in modifying evaporation rates and burning characteristics of palm-oil biodiesel droplets. It was found that, upon adding ethanol, the ignition delay and burn rate constant increased by 38.6% and 23.2%, respectively; however, the evaporation duration and burning period decreased by 20.6% and 22.5%, respectively. Viswanathan and Paulraj [18] studied the emission characteristics and performance of a diesel engine with different blends of diesel, jojoba oil, biodiesel, and butylated hydroxyl anisole.

The main focus of this study is to evaluate the chemical composition and combustion properties of jojoba-derived biodiesel, and also, to explore its benefits by testing it in CI engines. To the best of our knowledge, there is limited literature available on a comprehensive study of the ignition delay time (IDT), derived cetane number (DCN), and their temperature-dependent behavior compared directly with standard petrodiesel. The molecular composition of the fuel was characterized by using gas chromatography-mass spectrometry (GC-MS), and nuclear magnetic resonance (NMR). Its ignition characteristics were evaluated under engine-relevant conditions using the ignition quality tester (IQT). The findings presented demonstrate improved ignition quality and cleaner combustion characteristics, further solidifying the potential of jojoba biodieselas a sustainable alternative fuel for diesel engines.

2 Experimental approach

2.1 Preparation of jojoba biodiesel

Unrefined, organic, and cold-pressed jojoba oil from Leven Rose, Colorado, USA, was used to produce biodiesel. In this study, the alkali transesterification method was used to produce biodiesel. The free fatty acid content in the oil was assessed through standard titrimetry [19]. Methanol (molar mass 32.04 g mol^{-1}; boiling point 64.7 °C) and sodium hydroxide (molar mass 40.0 g mol^{-1}; melting point 323 °C; boiling point 1388 °C) served as the reactants and catalyst for the transesterification process. The oil was preheated at 100 °C for 60 min. The sodium methoxide solution prepared by dissolving sodium hydroxide in methanol is strongly alkaline, typically with a pH of 12–14, which ensures the catalytic activity required for the transesterification reaction. Biodiesel production was conducted in two batches. In the first batch, the residence time varied between 15 to 80 min while maintaining a constant CH_3OH-to-jojoba oil molar ratio of 8:1. The catalyst was dissolved in CH_3OH inside a round-bottom flask to form CH_3ONa, which was subsequently introduced into a three-neck sealed flask containing jojoba oil. The reaction mixture was stirred for different durations before being transferred to a separation funnel for glycerin removal (stage 2). In stage 3, the biodiesel layer was washed with distilled water and left to settle, forming two distinct layers. The upper phase contained biodiesel, while the lower phase consisted of methanol and residues. In stage 4, the biodiesel was subjected to further heating to eliminate any remaining water and methanol traces. The illustration has been given in Supplement (Fig. S1). For the second batch, the same procedure as batch 1 was followed, but with a fixed reaction time and a constant alcohol-to-oil molar ratio. The reaction temperature varied between 25 °C and 80 °C. The biodiesel yield from both stages was determined using volume percent, as calculated by Eq. (1) [20]. The Jan Warn Quist or 3/27 test was used to verify the completion of the reaction and to detect any unreacted triglycerides in biodiesel.

$$\text{Yield, \%} = \frac{\text{Volume of biodiesel}}{\text{Total feed volume }\left(\text{Oil} + \text{Methanol}\right)} \times 100 \quad (1)$$

2.2 Nuclear magnetic resonance spectroscopy

A 0.6 mL sample of the fuel mixture was prepared in 5 mm NMR tubes. The mixture contained 50 µL of the fuel (either jojoba crude oil or jojoba biodiesel) mixed in 1 mL $CDCl_3$. The NMR spectra were acquired at ambient temperature using a Bruker 700 AVANCE III spectrometer fitted with a Bruker CP TCI multinuclear CryoProbe (BrukerBioSpin, Rheinstetten, Germany). The ^1H NMR spectra were recorded with approximately 130 scans and a recycle delay of about 5 s, using a standard 1D 90° pulse sequence (zg) from the Bruker pulse library. Tetramethylsilane (TMS) was applied as the internal reference for chemical shift calibration. The spectral width was set to 14,098 Hz and digitized into 64k data points to capture the free induction decay. The ^{13}C NMR spectra were obtained using a 1D sequence with power-gate decoupling, a 30° flip angle, and a spectral width of 240 ppm. The data were collected as 64k complex points, with a 5-second recycle delay and 12k transients recorded per spectrum. Prior to the Fourier transformation, a 1 Hz exponential line broadening was applied. The 2D ^1H–^{13}C HMBC spectrum was recorded using the Bruker pulse sequence (hmbcgpl2ndqf) from the pulse library. The spectral width for the F_1 dimension was 42,255 Hz, while for the F_2 dimension, it was 11,160 Hz. HMBC data were acquired in absolute-value mode with a recycle delay of 3.0 s, using 4096 data points in t_2 and 512 data points in t_1 increments, with 48 scans per increment. The NMR spectra were recorded and analyzed using Bruker Topspin 2.1 software (BrukerBioSpin, Rheinstetten, Germany). A comparable methodology was followed in Elbaz et al. [19].

2.3 Gas chromatography and mass spectrometry

The qualitative analysis of liquid samples was conducted using a THERMO Trace GC Ultra system coupled with an MS DSQ II detector, equipped with a flame ionization detector (FID) for quantifying the principal components identified in the chromatograms. Prior to injection, the liquid samples were filtered and diluted tenfold with methanol (1:10). Separation was achieved on a DB-Petro capillary column using helium as the carrier gas at a flow rate of 2.3 mL min^{-1}. The oven temperature program began at 40 °C and was held for 4 min, followed by heating at 1 °C min^{-1} up to 55 °C, then at 2 °C min^{-1} to 185 °C, and finally at 10 °C min^{-1} to reach 250 °C, where it was maintained for 60 min. The injector, ion source, and transfer line temperatures were set at 300 °C, 230 °C, and 280 °C, respectively. A 1 µL aliquot of the sample was introduced into the system in split mode (1:7). A solvent delay of 8 min was applied before acquiring mass spectra. Data were collected in full-scan mode with a scan rate of 1600 μs^{-1}, and the detector voltage was adjusted to 1275 V to generate total ion chromatograms (TICs). Identification of compounds was carried out by matching the obtained mass spectra against entries in the National Institute of Standards and Technology (NIST) spectral library.

2.4 Ignition delay time and derived cetane number

The autoignition quality of the fuel in it governs combustion processes in diesel engines [21–24]. The cetane number (CN) of diesel-like fuels determines autoignition. The CN is traditionally measured in a cooperative fuel research (CFR) cetane engine by comparing its ignition qualities with reference fuels. The reference fuels are usually blends of highly reactive n-cetane or n-hexadecane and highly branched heptamethyl nonane. The reactive component is assigned a CN of 100, while heptamethyl nonane is given a CN of 15. This procedure is well explained in the paper by Kalghatgi [25]. The IQT has recently been used by Bogin et al. [21, 26–28]; Agarwal [1] and Naser et al. [29, 30] to measure the autoignition quality of diesel fuels using a standard test method, ASTM D6890-03a [31]. The IQT [29, 32] is a constant-volume combustion chamber with a spray injection system that measures the IDT of liquid sprays, including low-volatility fuels such as diesel and biodiesel. Temperature and pressure inside the chamber are maintained at around 815 K (541.85 °C) and 2.13 MPa, respectively. The small fuel mass requirement in the IQT makes it suitable for measuring IDT of fuels that are not available in large quantities. IDT in the IQT is defined as the time interval between the start of fuel injection into the chamber to the start of considerable heat release, where an average of 32 firing is recorded. The DCN or CN can be calculated using the measured IDT according to Eq. (2) [26, 29, 32].

$$\text{DCN} = 3.547 + 83.99 \times \left(\text{IDT} - 1.512\right)^{-0.658} \qquad (2)$$

Due to its experimental repeatability, the DCN measurement in the IQT is becoming increasingly preferred over the traditional CN measurement in the CFR. The King Abdullah University of Science and Technology (KAUST) IQT is used in this study to measure the IDT and DCN of the produced biodiesel (PB) at different charge temperatures. IDT and DCN measurements were also carried out for the crude jojoba oil and a US 2D petro-diesel. The results will help understand how the PB compares with the petrodiesel and crude jojoba oil.

3 Results and discussion

3.1 Jojoba crude oil

3.1.1 Physical properties and elemental composition of jojoba oil

The physical characteristics and elemental composition of jojoba oil have been investigated using conventional techniques. The physical and chemical composition of the oil used in this study is compared with characterization results from the literature on an Egyptian-grown jojoba oil to understand how the oil source affects its properties. The result is shown on Table 1. The measured density of the sample used in this study is 912.57 kg m^{-3}; slightly lower than the values reported by Shehata and Razek [6] (920 kg m^{-3}). The viscosity of jojoba oil at 40 °C, is around 31.56 mm^2 s^{-1}. This value is lower than the values reported by Shehata and Razek [6] (52 mm^2 s^{-1}) at similar temperature. The viscosity of a fuel increases as the molar mass increases and decreases by increasing the unsaturation level and temperature. The comparatively low viscosity value of jojoba oil used in this study can enhance mixing of the reactants during the esterification process. In addition, the low viscosity of the jojoba oil can reduce the difficulty in separating the PB from the glycerin during processing and ultimately improve the yield of jojoba biodiesel (methyl ester) [20]. The C/H ratio in this study is higher than that reported by Shehata and Razek [6]. Oxygen content of the jojoba oil in this study is higher than that of [6]. A characteristic aspect of the jojoba oil used here is the absence of sulfur in the oil. Higher C/H ratio, oxygen content, and the absence of sulfur in the oil sample used in this study might play a role in dictating the combustion and emissions characteristics of the oil sample used here, as compared to the jojoba oil used by Shehata and Razek [6]. The desulfurization process is often difficult and the presence of sulfur in hydrocarbon fuels is one of the major causes of environmental pollution. It can even cause harmful corrosion to the engine.

Table 1 Physical and elemental composition of jojoba crude oil

Property	Our study	Shehata and Razek [6]
Density (kg m^{-3})	912.57	920
Viscosity (mm^2 s^{-1})	31.56	52
C (wt.%)	77.61	81.36
H (wt.%)	11.46	12.94
O (wt.%)	10.41	5.7
N (wt.%)	0.51	0
S (wt.%)	0	0.02
Heating value (MJ kg^{-1})	39.42	39.86

3.1.2 Gas chromatography and mass spectrometry of jojoba oil

The GC-MS was used to study the chemical composition of the crude jojoba oil. Different components were detected at various retention times. The gas chromatogram of the jojoba oil is shown in Fig. 1. Table 2 shows the main compounds identified by the GC-MS, indicating the presence of several fatty acid methyl esters (FAMEs) and long-chain esters typical of jojoba oil. The percentage areas of peaks 1–5 of jojoba oil were 49.4, 21.2, 12.0, 4.91, and 3.61, respectively; moreover, the corresponding retention times were 39.8, 35.8, 24.4, 14.2, and 33.7. The main compounds identified are linoleic acid (C18:2), oleic acid (C18:1), palmitic acid (C16:0), methyl linoleate (C18:2), stearic acid (C18:0). These are all high molar mass oxygenated compounds. Usually, typical biodiesel is made of a mixture of FAMEs derived from these compounds [33, 34]. In addition, the numbers before and after the colon symbol (:) represent the amount of carbon atoms and carbon double bonds in the respective fatty acids [35].

3.1.3 ^{1}H and ^{13}C NMR analysis of jojoba oil

The ^{1}H NMR and the ^{13}C NMR spectra of the crude jojoba oil are shown in Tables 3 and 4, respectively. The jojoba oil consists of several molecules, which makes it difficult to determine the structure of all the molecules. Therefore, the chemical shifts are used to identify and quantify different structure groups in the oil sample. Tables 3 and 4 show the chemical shifts used for different structure groups and their corresponding mole percentages calculated after integrating the baseline corrected spectrum of the ^{1}H NMR and ^{13}C NMR. ^{1}H NMR results show that the crude oil contains a large amount of aliphatic H atoms (CH_2, CH_3), a relatively low amount of olefinic H atoms (~10%), epoxide/glyceridic H atoms (3.86%), and a negligible amount of carboxylic hydrogen. The ^{13}C NMR spectra in Table 4 indicated the presence of four different types of C atoms. The results showed that the jojoba oil sample contains a high amount of aliphatic carbon (~72%), approximately 18% olefinic carbon, and relatively low quantities of carboxylic carbon and glyceridic carbon groups. Interestingly, although 5.64% of the C atoms are carboxylic, only 0.04% of H atoms are carboxylic.

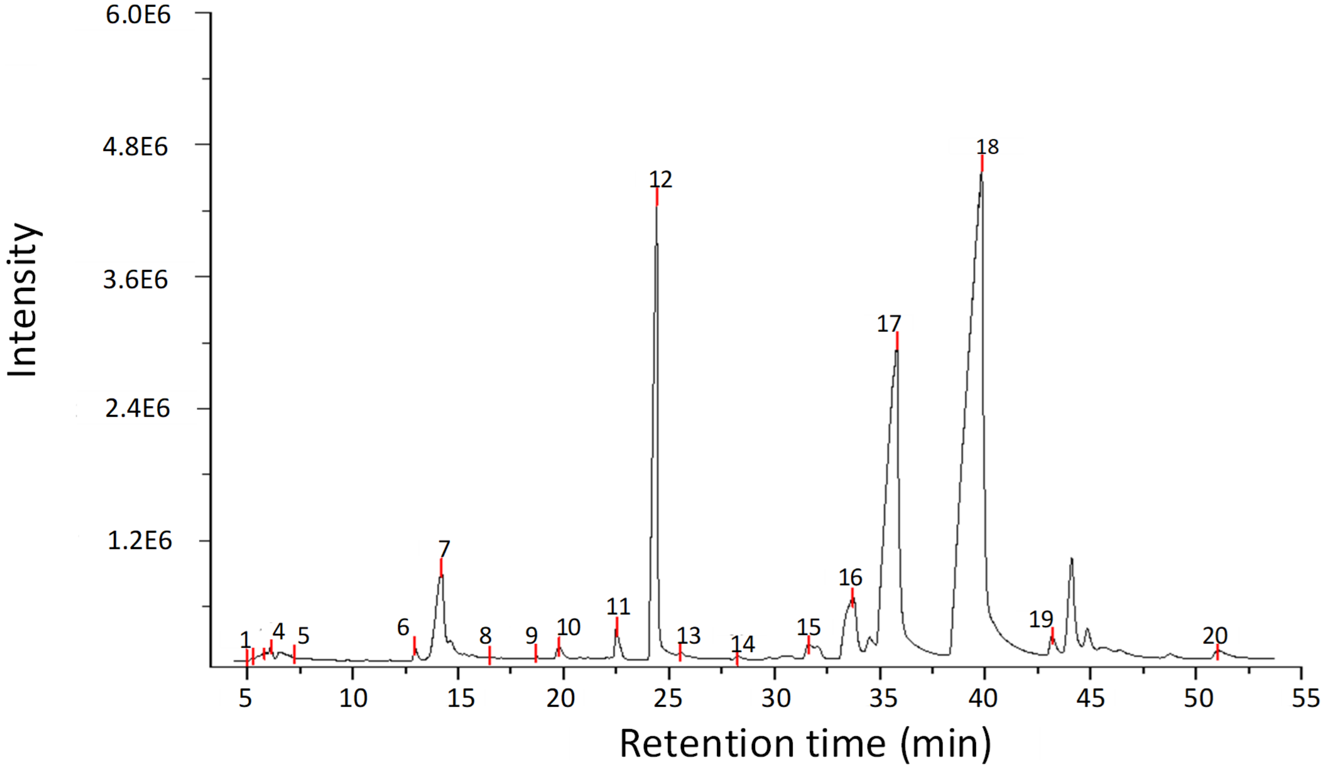


Fig. 1 GC-MS analysis of crude jojoba oil showing major fatty acid components

3.2 Jojoba biodiesel

3.2.1 Physical properties and elemental composition of jojoba biodiesel

As mentioned earlier, the composition of the extracted biodiesel depends on the crude oil source and on the transesterification process. The jojoba PB was also characterized to determine its physical and chemical characteristics. The values obtained from this study were compared with literature values and ASTM standard values for biodiesels. The result is shown in Table 5 [4, 5, 13, 36, 37]. The measured density of the biodiesel in this study is 870 kg m^{-3}, comparable to the values reported by [4, 36]. This value also falls within the range of the standard values for Biodiesel fuel. The viscosity of the PB is 4.21 mm^2 s^{-1}, within the range of the standard values. The viscosities reported by [4, 36] are slightly higher than our values. The viscosity value of fuel shows its ability to flow. High-viscosity fuels are difficult to atomize, leading to reduced thermal efficiency and increased soot deposits. The comparatively low viscous biodiesel produced in this study means smaller fuel droplets, better vaporization, and delivery into the combustion chamber. The weight percentage of carbon, hydrogen and oxygen of the PB compare well with the acceptable standard values. Table 6 presents the simulated distillation data, demonstrating the correlation between weight % and measured boiling point.

3.2.2 Gas chromatography and mass spectrometry analysis of jojoba biodiesel

The methyl ester content identified by GC-MS in the jojoba biodiesel is shown in Fig. 2 and Table 7 [38]. The main compounds identified are methyl linoleate (C18:2), methyl oleate (C18:1), methyl palmitate (C16:0), methyl linolenate (C18:3), methyl stearate (C18:0). methyl linoleate (C18:2) and methyl linolenate (C18:3) are polyunsaturated fatty acid esters, which generally exhibit better low-temperature fluidity, enhancing fuel performance in colder climates. However, their high degree of unsaturation can lead to oxidative instability, impacting storage and shelf life.

Due to moderate reactivity and balanced saturation level of methyl oleate (C18:1), it contributes to good ignition quality, stability, and efficient combustion. Methyl palmitate (C16:0) and methyl stearate (C18:0), both saturated fatty acid esters, improve oxidative stability, CN, and overall combustion characteristics. However, they can impact low-temperature operability due to their higher melting points. The stability of biodiesel mainly depends on the degree of unsaturation present in the FAMEs [39, 40]. Thus, the major compounds identified in the PB (methyl linoleate, methyl oleate, methyl palmitate, methyl linolenate, and methyl stearate) have varying impacts on oxidative stability. Polyunsaturated compounds such as methyl linoleate (C18:2) and methyl linolenate (C18:3),

Table 2 Main compounds in jojoba oil identified by GC-MS

Peak number	Retention time (min)	% Area	Compound
1	39.8	49.4	(Z,Z)-9,12-Octadecadienoic acid (linoleic acid, C18:2) $C_{18}H_{32}O_2$ CAS no. 60-33-3
2	35.8	21.2	(E)-9-Octadecenoic acid (oleic acid, C18:1) $C_{18}H_{34}O_2$
3	24.4	12.0	n-Hexadecanoic acid (palmitic acid, C16:0) $C_{16}H_{32}O_2$ CAS no: 57-10-3
4	14.2	4.91	(E,E)-9,12-Octadecadienoic acid, Methyl ester (methyl linoleate, C18:2) $C_{19}H_{34}O_2$
5	33.7	3.61	Octadecanoic acid (stearic acid, C18:0) $C_{18}H_{36}O_2$ CAS no: 57-11-4
6	4.97	0.006	2-Octenoic acid [$C_8H_{14}O_2$]. CAS no: 1470-50-4
7	5.30	0.008	2-Hydroxy-2-methyl-butanoic acid methyl ester [$C_5H_{10}O_3$]. CAS no: 3739-30-8
8	5.81	0.035	β-Citronellol (3,7-dimethyl-6-octen-1-ol) [$C_{10}H_{20}O$]. CAS no. 106-22-9
9	6.11	0.165	1-Hexyl-2-nitrocyclohexane [$C_{12}H_{23}NO_2$]
10	7.24	0.012	(Z)-4-Decen-1-ol [$C_{10}H_{20}O$] CAS no: 57074-37-0
11	12.9	0.293	Glycerin [$C_3H_8O_3$] CAS no: 56-81-5
12	16.9	0.018	Glycerol 1-myristate [$C_{17}H_{34}O_4$] CAS no: 1330-67-2
13	18.7	0.066	2-(Aminooxy)-propanoic acid [$C_3H_7NO_3$] CAS no: 2786-22-3
14	19.8	0.426	Mono-methyl sebacate (10-Methoxy-10-oxodecanoic acid) $C_{11}H_{20}O_4$ CAS no: 818-88-2
15	22.5	0.780	3-(Dimethylamino)-2-propenoic acid, methyl ester [$C_6H_{11}NO_2$]
16	25.6	0.079	3-Methyl-heptanedioic acid, dimethyl ester ($C_{10}H_{18}O_4$) CAS no: 54576-14-6
17	28.3	0.110	D-(-)-Ribose ($C_5H_{10}O_5$) CAS no: 10257-32-6
18	31.6	1.05	Monomyristin ($C_{17}H_{34}O_4$) CAS no. 589-68-4
19	43.2	0.611	(-)-Isolongifolol ($C_{15}H_{26}O$). CAS no. 1139-17-9
20	51.1	0.512	1-Tridecyne ($C_{13}H_{24}$). CAS no: 26186-02-7

Table 3 Hydrogen types in jojoba oil

Hydrogen type	Chemical shift (ppm)	Peak area	Mol %
Aliphatic CH_3	0.7–1	535380545.5	8.91
Aliphatic CH_2	1.1–3	4629867632.0	77.03
Epoxide/Glyceridic group	4.1–4.4	231787756.7	3.86
Olefinic hydrogen	5.2–5.5	611105979.4	10.17
Carboxylic hydrogen	7.2–7.3	2525751.95	0.04
Total		6010667666	100.00

Table 4 Carbon types in jojoba oil

Carbon type	Chemical shift (ppm)	Peak area	Mol %
Aliphatic carbon	13.8–38	682514155.1	71.83
Epoxide/Glyceridic group	60–70	45364133.4	4.77
Olefinic carbon	125–133	168634442.3	17.75
Carboxylic carbon	170–175	53605800.3	5.64
Total		950118531.1	100

despite providing desirable low-temperature fluidity, are more prone to oxidation due to their higher unsaturation levels, potentially leading to fuel degradation, increased acidity, formation of gums, sediments, and changes in fuel color over storage periods.

Table 5 Physical properties and elemental composition of biodiesel

Property	Value from this study	Values from literature	ASTM D6751-24 [37] biodiesel
Density (kg m^{-3})	870	866.6 [4], 830 [5], 871.6 [36]	860–900 [5]
Viscosity (mm^2 s^{-1})	4.21	19.2 [4], 2.2 [5], 10.44 [36]	1.9–6.0 [5]
C (wt.%)	76.36	87	77 [13]
H (wt.%)	11.67	13	12 [13]
O (wt.%)	11.3		11 [13]
N (wt.%)	0.66		
S (wt.%)	0		0.05 [5]
Heating value (MJ kg^{-1})	39.76	47.38 [4], 35.66 [36]	

Table 6 Simulated distillation (GC)

%Mass	Boiling point measured (°C)
0	113.9 = 387.05 K
5	166.2 = 439.35 K
10	187.8 = 460.95 K
20	217.0 = 490.15 K
30	238.9 = 512.05 K
40	257.6 = 530.75 K
50	273.7 = 546.85 K
60	289.5 = 546.85 K
70	304.5 = 577.65 K
80	319.5 = 592.65 K
90	338.3 = 611.45 K
95	349.4 = 622.55 K
100	367.4 = 640.55 K

3.2.3 ^{1}H and ^{13}C NMR analysis of jojoba biodiesel

The ^{1}H NMR and the ^{13}C NMR spectra of the biodiesel derived from the crude jojoba oil are shown in Tables 8 and 9, respectively. ^{1}H NMR results show that the biodiesel fuel contains a large amount of aliphatic H atoms CH_2 (~73%) and CH_3 (~9%), a relatively low amount of olefinic and methoxide H atoms (~8% each), and a negligible amount of carboxylic hydrogen. The ^{13}C NMR spectra in Table 9 show four different types of C atoms. The results showed that the biodiesel fuel contains a high amount of aliphatic carbon (~70.5%), olefinic carbon (~19%), and a relatively low amount of olefinic and methoxide C atoms (~5% each).

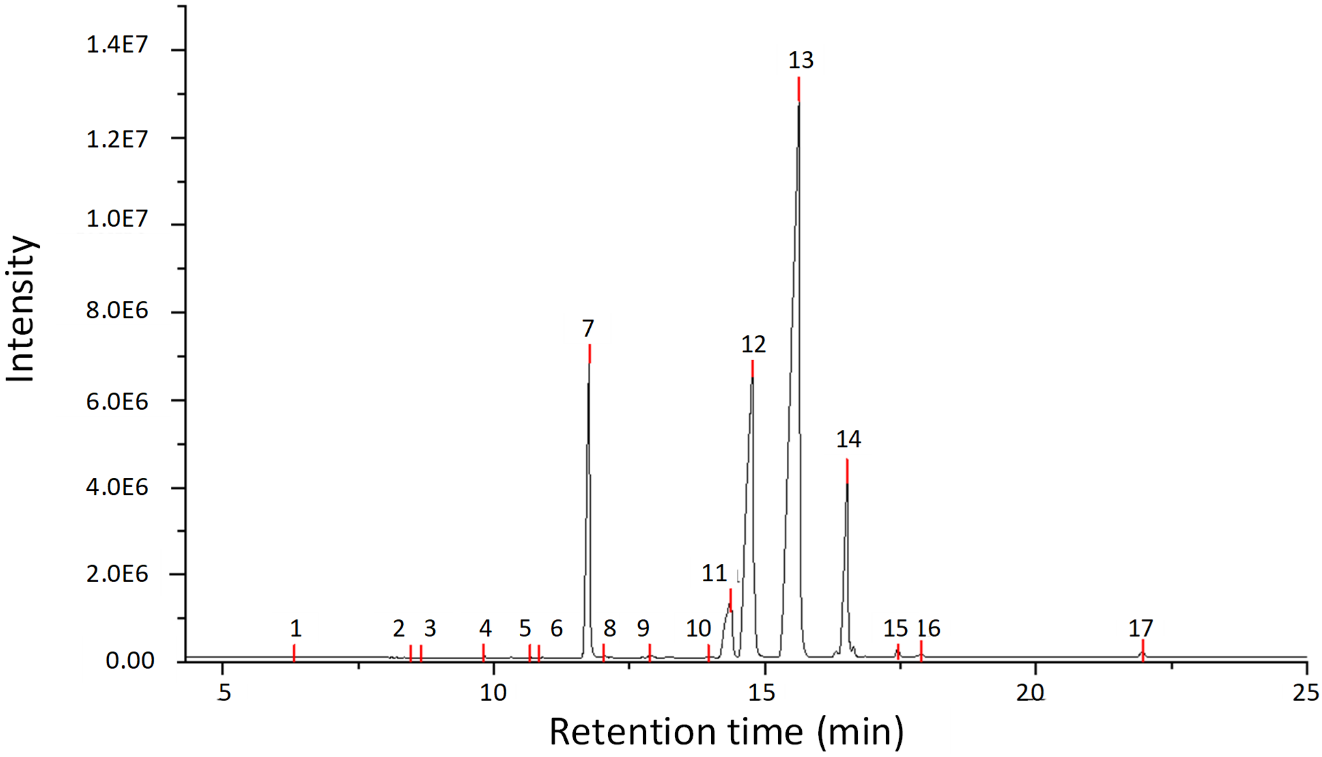


Fig. 2 GC-MS chromatogram of jojoba-derived biodiesel, highlighting the primary fatty acid methyl esters

Table 7 Main compounds identified by GC-MS in the produced jojoba biodiesel

Peak number	Retention time (min)	% Area	Identified compound
1	15.63	54.61	Methyl linoleate (C18:2, methyl ester of linoleic acid)
2	14.77	23.94	Methyl oleate (C18:1, methyl ester of oleic acid)
3	11.76	11.62	Methyl palmitate (C16:0, methyl ester of palmitic acid)
4	16.51	8.57	Methyl linolenate (C18:3, methyl ester of linolenic acid)
5	14.37	5.46	Methyl stearate (C18:0, methyl ester of stearic acid)

Table 8 Hydrogen types in the produced biodiesel

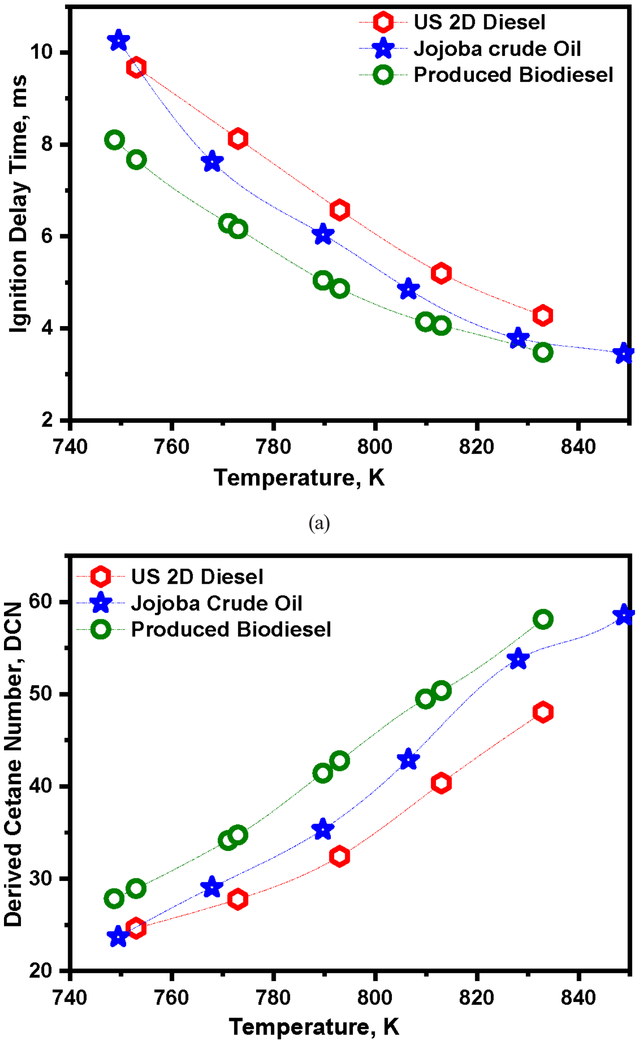
Hydrogen type	Chemical shift (ppm)	Peak area	Mol %
Aliphatic CH_3	0.7–1.1	397166774.6	9.38
Aliphatic CH_2	1.1–3	3104639683	73.32
Methoxide group	3.65–3.66	368789629.6	8.71
Olefinic hydrogen	5.2–5.5	362164541.4	8.55
Carboxylic hydrogen	7.2–7.3	1507119.07	0.04
Total		4234267747	100

Table 9 Carbon types in the produced biodiesel

Carbon type	Chemical shift (ppm)	Peak area	Mol %
Aliphatic carbon	13.8–38	629421415.1	70.45
Methoxide group	51.3	45955868.2	5.14
Olefinic carbon	125–133	170619462.8	19.10
Carboxylic carbon	170–175	47442192.28	5.31
Total		893438938.3	100

3.3 Ignition quality tester analysis of jojoba oil, jojoba biodiesel and US 2D petro-diesel

IDT is the time between the start of fuel injection to the beginning of combustion, which occurs through fuel atomization, vaporization, and fuel–air mixing [41, 42]. Fig. 3 (a) shows the IDT of the tested fuels at different charge temperatures. It was also observed that the PB shows shorter IDT than jojoba crude oil and US 2D diesel. This may be due to a rapid preflame chemical reaction that occurs at high temperatures. Due to his high temperature reaction, biodiesel may experience thermal cracking, and lighter compounds are produced, which may ignite earlier and shorten the IDT [43, 44]. Fig. 3 (b) exhibits the relation between DCN and temperature for three test fuels. It was shown that DCN increases with increasing temperature for all three fuels (US 2D diesel, jojoba crude oil, and the PB). It was also observed that the PB has a higher DCN than jojoba crude oil and US 2D diesel. Typically, biodiesel has a higher CN than diesel [45]. The IDT graph (Fig. 3 (a)) exhibited the shorter IDT for all temperatures. This trend is directly correlated with the higher DCN in Fig. 3 (b). Thus, biodiesel's higher DCN validates its superior ignition reactivity compared to jojoba crude oil and diesel. IDT is a fundamental parameter for validating chemical kinetic models, as it reflects the combined effects of all chemical processes involved in combustion and product formation [46]. The CN and ignition quality were enhanced, thereby improving the combustion efficiency and reducing emissions.



(a)

(b)

Fig. 3 Comparison of (a) ignition delay time and (b) derived cetane number of the tested fuels at different ambient temperatures

4 Conclusions

An experimental evaluation including production, characterization, and combustion properties of biodiesel produced from jojoba oil has been conducted in the current study. It was found that the density (870 kg m^{-3}), viscosity (4.21 mm^2 s^{-1}), composition of carbon (76.36%), hydrogen (11.67%) and oxygen (11.3%) of biodiesel are in accordance with ASTM D6751-24 [37]. It confirmed that the biodiesel has good flowability, atomization, efficient combustion and reduced soot formation during combustion. GC-MS analysis identified major components, including methyl linoleate, methyl oleate, and methyl palmitate, contributing to the biodiesel's high energy content of 39.76 MJ kg^{-1}. NMR analysis further confirmed the dominance of aliphatic hydrogen and carbon. Moreover, the jojoba oil-derived biodiesel is sulfur-free, which eliminates sulfur oxide emissions and reduces environmental and engine-related issues. In addition, the IQT analysis showed superior ignition quality, with a higher DCN and shorter IDT than US 2D diesel and crude jojoba oil, which indicates its suitability for diesel engine applications.

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Abbreviations

ASTM	American Society for Testing and Materials
CFR	cooperative fuel research
CI	compression ignition
CN	cetane number
DCN	derived cetane number
FAAEs	fatty acid alkyl esters
FID	flame ionization detector
GC-MS	gas chromatography-mass spectrometry
ID	ignition delay
IDT	ignition delay time
IQT	ignition quality tester
KAUST	King Abdullah University of Science and Technology
NIST	National Institute of Standards and Technology
NMR	nuclear magnetic resonance
PB	produced biodiesel
SCM	supercritical methanol
SI	spark ignition
TICs	total ion chromatograms
TMS	tetramethylsilane

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