

Jojoba Biodiesel Transesterification: An Experimental Study and Short Path Distillation Model in Aspen HYSYS

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Abstract

The transition to sustainable energy requires exploring non-edible feedstocks like Jojoba oil. However, its long-chain wax esters present severe physical separation challenges during conventional biodiesel production. This study investigates crude Jojoba oil transesterification through an integrated experimental and computational approach. Laboratory experiments, utilizing a 6:1 methanol-to-oil molar ratio and a sodium carbonate catalyst at 50 °C, achieved a 91.3% reaction efficiency. Nevertheless, separating the resulting methyl esters was hindered by persistent waxy emulsions caused by long-chain wax esters (Eicosanol), making standard gravity decanting inadequate. To overcome this limitation, a digital twin was developed using Aspen HYSYS with the Non-Random-Two-Liquid thermodynamic package. Modeling Jojoba as a hypothetical component, the simulation implemented Short Path Distillation operating under extreme vacuum conditions (0.1 kPa). The model successfully separated the complex mixture, predicting an exceptional methyl ester purity of 97.17% and an overall mass yield of 98.2%. The process achieved an 83.1% recovery rate of unreacted methanol and produced a biodiesel stream with a kinematic viscosity of 7.758 cSt at 40 °C. Although this viscosity slightly exceeds the ASTM D6751 upper limit due to the unique long-chain wax ester composition inherent in Jojoba oil, it can be effectively optimized through fuel blending strategies. Ultimately, integrating high-vacuum thermal separation provides a scalable industrial solution to Jojoba's separation bottlenecks, yielding premium biofuel and lucrative fatty alcohols.

Keywords:

Jojoba oil, Biodiesel, Transesterification, non-edible oil, Aspen HYSYS, Short path distillation, Biomass energy, Renewable energy.

1. Introduction

Addressing the current global environmental crisis caused by energy production, biodiesel has emerged as a significant research focus due to its potential as a renewable, cost-effective, and eco-friendly fuel [1, 2]. Biodiesel offers distinct environmental advantages, primarily through cleaner exhaust emissions that significantly reduce the release of harmful pollutants compared to conventional diesel. It is also highly biodegradable and non-toxic, making it safer for ecosystems [3, 4]. Transesterification of a vegetable oil was conducted as early as 1853 by Patrick Duffy, four decades before the first diesel engine became functional [5]. Transesterification is a chemical process in which the hydroxyl group of an alcohol reacts with the carboxylic group of triglycerides, resulting in the formation of ester compounds [6, 7].

The transesterification process is a complex chemical reaction governed by several interconnected parameters. Primarily, the choice of catalyst whether homogeneous or heterogeneous is crucial for achieving efficient conversion [8, 9, 10]. In tandem with the catalytic system, the reaction temperature acts as a

fundamental thermodynamic variable. For the majority of vegetable oil feedstocks reacting with methanol, the optimal thermal window is generally identified between 50 °C and 60 °C. Maintaining this specific range is critical; operating below these temperatures significantly increases both the activation energy requirements and liquid viscosity, thereby hindering the reaction rate [11, 12].

Furthermore, the alcohol-to-oil molar ratio serves as a key stoichiometric determinant that dictates the complete synthesis of methyl esters [12]. This ratio must be carefully optimized alongside the chosen catalyst to ensure maximum conversion efficiency. Beyond these operational variables, the inherent chemical composition of the feedstock, particularly the presence of Free Fatty Acids (FFAs), poses a significant technical challenge. In alkaline-catalyzed transesterification, excess FFAs trigger an undesirable saponification reaction. This side reaction not only produces soap and excessively consumes the catalyst, but it also leads to increased viscosity and the formation of stable emulsions. Consequently, these emulsions severely hinder the phase separation between methyl esters and glycerol, ultimately reducing overall yields and complicating downstream purification [7, 13].

Bouaid et al. [14] investigated jojoba oil as a promising non-edible feedstock, achieving an 83.5% ester yield at 25 °C with a 1.35% catalyst concentration. They noted that higher temperatures and catalyst levels caused negative synergistic effects due to saponification, while also confirming that the biodiesel's fuel properties met the required standards and emphasizing that economic viability depends on co-producing valuable fatty alcohols. Expanding on catalyst optimization, Shah et al. [15] demonstrated that synthesizing biodiesel from non-edible jojoba oil using an optimized organotin catalyst achieves an exceptional 92.6% yield, significantly outperforming standard base catalysts. The resulting biofuel is highly important as a sustainable energy alternative because its physical properties strictly comply with international ASTM D6751 standards. This confirms that jojoba oil is a highly viable and reliable feedstock for producing premium-quality, commercial grade biodiesel, Abdelmoez et al. [16] investigated biodiesel synthesis from jojoba oil extracted via eco-friendly subcritical water technology. By optimizing the base-catalyzed transesterification process, they identified a 6:1 methanol-to-oil molar ratio, a 1.35 wt% KOH catalyst concentration, and 600 rpm stirring as the ideal operating parameters. The study concluded that temperature critically dictates reaction kinetics; operating at 50 °C maximized efficiency, achieving a 95% conversion rate in just 25 minutes. Conversely, lower temperatures significantly hindered both speed and yield, dropping to 87% at 40 °C (50 minutes) and 83% at 25 °C (80 minutes), emphasizing the necessity of optimal thermal control, further, Al-Shanableh et al. [17] demonstrated the efficiency of the supercritical methanol (SCM) method for jojoba biodiesel production, achieving a 97.8% conversion yield at 240 °C and 8.3 MPa. While the resulting fuel met standard kinematic viscosity limits, the study significantly highlighted the inherent physical challenge posed by jojoba's unique "liquid wax" composition. The authors explicitly noted that because of this waxy nature, the reaction inherently produces a challenging mixture of methyl esters (FAME) and heavy fatty alcohols, rather than pure biodiesel. This complex composition not only elevates the cold flow properties but also distinctly underscores the critical, unresolved need for advanced separation technologies to successfully isolate the pure biofuel from these heavy alcoholic byproducts. The study concluded that SCM provides a superior, catalyst-free alternative to conventional methods, offering rapid, high-purity sustainable fuel production. Recently, Abdulrahman and Al-Ahmadi [18] investigated the alkali-catalyzed transesterification of unrefined jojoba oil, optimizing the process using an 8:1 methanol-to-oil molar ratio, NaOH catalyst, and varying temperatures (25–80 °C) and residence times (15–80 minutes). The synthesized biofuel, predominantly composed of long-chain fatty acid methyl

esters, strictly complied with ASTM D6751-24 standards, exhibiting an ideal density of 870 kg/m³ and a kinematic viscosity of 4.21 mm²/s. Crucially, combustion analysis demonstrated that this sulfur-free biodiesel possesses superior ignition reactivity evidenced by a higher derived cetane number and shorter ignition delay compared to standard petro diesel, establishing it as a highly efficient and promising alternative fuel.

Despite these highly successful chemical conversions, the unique nature of jojoba oil presents severe physical separation challenges downstream. Sánchez et al. [19] provided a detailed review emphasizing that jojoba oil consists almost entirely of long-chain wax esters rather than standard triglycerides. They noted that the reaction produces valuable but problematic heavy jojobyl alcohols instead of a distinct liquid glycerin layer, making final product purification exceedingly difficult when utilizing standard catalysts. Supporting this operational concern, Malabadi et al. [20] highlighted that while homogeneous catalysts offer fast reaction rates, they severely complicate product separation, cause equipment corrosion, and often lead to the formation of stable emulsions. Consequently, resolving these physical purification bottlenecks remains a critical hurdle for commercial scale-up.

To economically address these process limitations, researchers have increasingly relied on advanced process simulation. Karacan and Çağatay [21] successfully simulated the continuous reactive distillation of waste cooking oil using Aspen HYSYS, proving its effectiveness in evaluating key operating parameters and minimizing overall production costs. Similarly, Anam et al. [22] simulated continuous biodiesel production from waste cooking oil in Aspen HYSYS, identifying a 1:3 oil-to-methanol ratio at 385.4 K as optimal for a CaO-catalyzed process. Although their NRTL based model achieved a high purity of 99.09 wt%, the final product failed to strictly satisfy ASTM D6751 standards due to 0.91 wt% residual glycerol, despite the utilization of membrane separators. This limitation explicitly highlights the persistent purification bottlenecks associated with conventional triglyceride feedstocks, contrasting sharply with the unique separation dynamics required for wax ester-based oils.

Silva and Andrade [23] utilized Aspen Plus to simulate continuous biodiesel production from four standard vegetable oils, explicitly modeling the feedstocks using a mixed triglyceride approach. Under optimal CSTR conditions (60 °C, 6:1 methanol-to-oil ratio, and a 2-hour residence time), the methanolic transesterification achieved up to 93% conversion, producing a fuel that strictly complied with ASTM D6751 and EN 14214 standards. However, because this comprehensive simulation is fundamentally anchored in conventional triglyceride chemistry, it does not account for the unique wax ester composition of non-traditional feedstocks like jojoba, thereby leaving the complex physical separation of heavy fatty alcohol byproducts entirely unaddressed.

However, a comprehensive review of these studies reveals a significant research gap. While simulation tools have been extensively applied to standard triglyceride-based oils, the current literature lacks integrated Aspen HYSYS models dedicated to resolving the unique physical separation barrier of jojoba's waxy emulsions using advanced thermal solutions, such as Short Path Distillation.

This study aims to optimize biodiesel yield and develop a validated industrial simulation model. Operating under specifically defined parameters (crude jojoba oil, sodium carbonate catalyst, 6:1 molar ratio, and 50 °C), the research addresses the failure of conventional distillation columns by introducing an advanced Short Path Distillation (SPD) approach. By utilizing Aspen HYSYS V12 integrated with the NRTL thermodynamic package, this work fills a critical engineering gap, providing an accurate, scalable thermal solution for sustainable biofuel production.

2. Methodology:

This section outlines the systematic methodology employed to investigate the production and purification of biodiesel from crude jojoba oil. The research adopts a dual approach, integrating laboratory scale experiments with advanced process simulation. While the experimental phase focuses on the transesterification reaction and efficiency, the computational phase utilizes Aspen HYSYS to model the industrial scale-up, with a specific emphasis on overcoming separation challenges through Short Path Distillation (SPD).

2.1 Materials and Experimental Procedure:

The primary feedstock utilized in this study was crude jojoba oil. Before commencing the transesterification process, the raw oil was characterized by chromatographic analysis to establish a baseline for its chemical and physical behavior. The detailed Table 1: Physicochemical properties of crude jojoba oil presents these essential parameters, highlighting the oil's high initial viscosity and wax ester content which differentiate it from conventional vegetable oils.

Table 1. Physicochemical properties of crude jojoba oil

Parameter	Value	Unit
Specific Gravity	0.864	-
Refractive Index	1.4612	-
Iodine Value	82.63	g I ₂ /100g
Saponification Value	92.3	mg KOH/g
Acidity	0.23	%
Peroxide Value	02.01	meq/kg

The properties in Table 1 confirm the unique suitability of the crude jojoba oil for sustainable biodiesel production. Most notably, the exceptionally low saponification value (92.3 mg KOH/g) proves the feedstock consists primarily of long-chain wax esters rather than standard triglycerides. Furthermore, the minimal acidity (0.23%) eliminates the risk of severe soap formation, technically validating the implementation of a single-step, base-catalyzed transesterification process. Finally, the moderate iodine and low peroxide values indicate excellent feedstock freshness, ensuring strong oxidative stability for the resulting biofuel.

The experiment was conducted in duplicate to ensure accuracy. The results reported in this study are expressed as the mean value $\pm$ standard deviation (SD), calculated to evaluate the consistency and reproducibility of the experimental procedure at the laboratories of Omar Al-Mukhtar University, Libya. The process was carried out in a laboratory-scale glass batch reactor equipped with precision monitoring instruments. Initially, the homogeneous catalyst, sodium carbonate (Na₂CO₃), was accurately measured to 1.33 wt% using a digital analytical balance. The crude jojoba oil was then introduced into the reactor and preheated to a target temperature of 50 °C using a laboratory hot plate. The thermal state of the process was continuously monitored and regulated using a digital thermometer.

Upon reaching the desired temperature, methanol was added to achieve a precise 6:1 methanol-to-oil molar ratio. To ensure maximum mass transfer and physical contact between the reactants, the mixture was subjected to constant agitation using a magnetic stirrer for a residence time of 30 minutes. Figure 1 illustrates the complete experimental setup utilized for the transesterification of Jojoba oil.

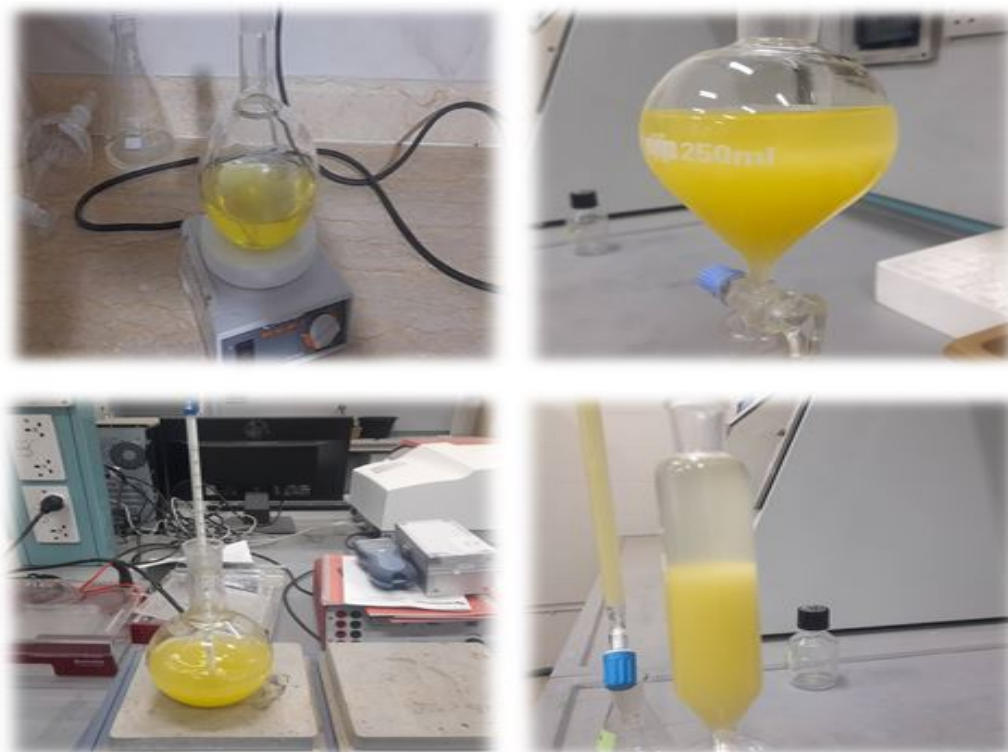


Fig 1. Experimental setup for the transesterification of Jojoba oil.

Following the reaction period, the mixture was allowed to settle undisturbed for 60 minutes to facilitate the initial physical phase separation. To ensure the removal of impurities and residual catalyst, the recovered biodiesel layer underwent a purification process consisting of water washing followed by gravity separation, which was repeated for three successive cycles. Subsequently, the final product was heated at 70 °C for 20 minutes to eliminate any remaining traces of moisture and unreacted methanol. These refined experimental procedures provided the necessary samples for physicochemical characterization and established the empirical baseline required to configure the advanced thermal separation model in Aspen HYSYS.

2.2 Process Simulation and Thermodynamic Modeling:

To extend the laboratory findings into a scalable industrial framework, a detailed process simulation model was constructed using Aspen HYSYS. This computational approach aims to evaluate the technical feasibility of Jojoba biodiesel production and to optimize the complex thermal separation required to handle waxy emulsions.

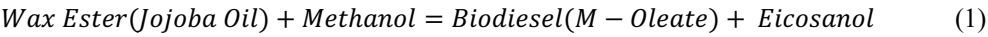
The simulation utilizes the Non-Random Two-Liquid (NRTL) thermodynamic fluid package. This choice is technically justified by the presence of highly non-ideal mixtures consisting of polar methanol and large, long-chain jojoba wax esters and alcohols. The NRTL model provides the necessary precision to calculate phase equilibrium and energy balances, particularly for the vacuum distillation stages where molecular interactions significantly deviate from ideal behavior.

The sodium carbonate (Na_2CO_3) catalyst was modeled as a component in the reaction set. To match our experimental outcomes, the reaction conversion efficiency was fixed at 95% within the Aspen HYSYS kinetic/conversion reactor model.

A critical step in the model's development was the characterization of Jojoba oil, which is not available in the standard HYSYS library. The oil was defined as a "Hypothetical Component" based on experimental data. While a theoretical molecular weight of 606 g/mol is often associated with pure Jojoba wax esters, this

study utilized a calibrated value of 563 g/mol. This adjustment was scientifically essential to align the simulation with the specific physicochemical profile of the crude Jojoba oil analyzed in Libya (Table 1). By refining the molecular weight to 563 g/mol, the model achieved a high-fidelity match with the measured mass density and boiling point characteristics, thereby ensuring the reliability of the subsequent separation calculations.

The chemical reaction used in the Aspen HYSYS reaction set is the transesterification of Jojoba wax esters with methanol, which produces methyl esters and Eicosanol. The stoichiometric reaction is explicitly defined as:



The complete integrated process flowsheet is presented in Figure 2. The model simulates the continuous transesterification reaction followed by a sequence of purification units designed to isolate high-purity methyl esters.

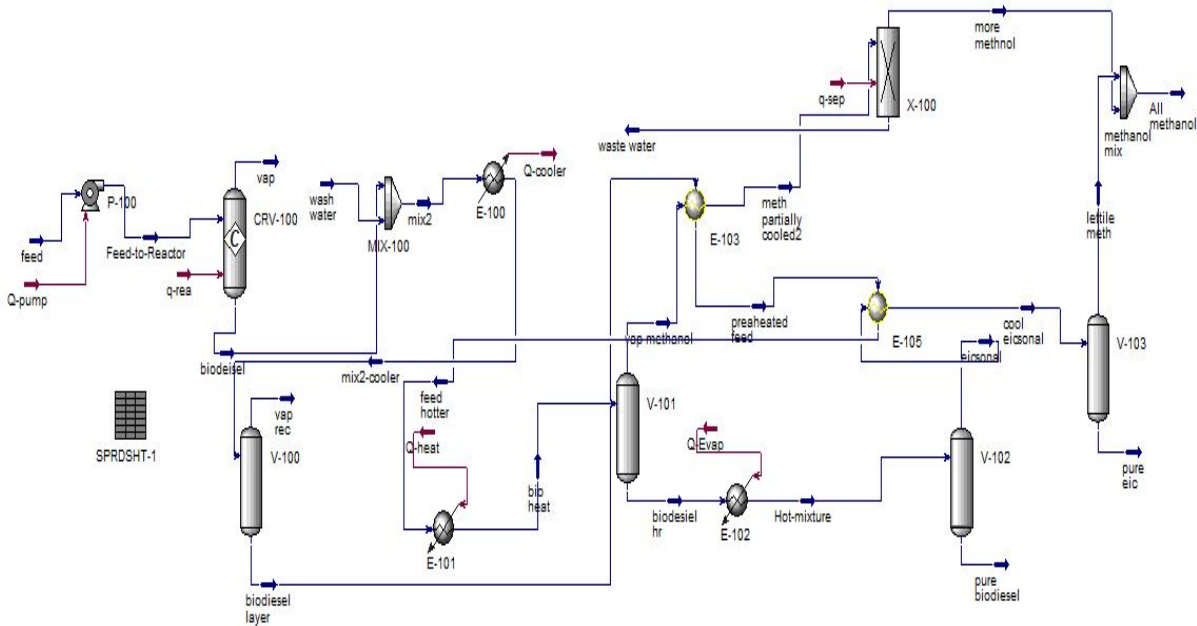


Fig 2. Comprehensive Aspen HYSYS flowsheet for Jojoba biodiesel production and purification.

To resolve the separation bottleneck identified during the experimental phase, the simulation incorporates a Short Path Distillation (SPD) unit, as shown in Figure 3. The SPD is the core engineering solution of this model, designed to fracture the biodiesel-alcohol-wax mixture.

Separator: V-102		
Design Reactions Rating Worksheet Dynamics		
Worksheet	Name	Hot-mixture
Conditions	Vapour	0.5472
Properties	Temperature [C]	200.0
Composition	Pressure [kPa]	0.1000
PF Specs	Molar Flow [kgmole/h]	30.88
	Mass Flow [kg/h]	8576
	Std Ideal Liq Vol Flow [m3/h]	10.14
	Molar Enthalpy [kJ/kgmole]	-5.309e+005
	Molar Entropy [kJ/kgmole-C]	823.8
	Heat Flow [kJ/h]	-1.639e+007

Fig 3. SPD conditions.

The unit was configured to operate under an extreme vacuum of 0.1 kPa to significantly lower the boiling points of the heavy components and prevent thermal degradation. The specific operational parameters and the output conditions generated by the simulation are summarized in Table 2.

Table2. Input Data and the output conditions.

Name	Temperature	Pressure
<i>Unit</i>	<i>°C</i>	<i>kPa</i>
feed	50	100
vap	50	200
biodiesel	50	200
vap rec	30	200
wash water	50	200
mix2	50	200
Feed-to-Reactor	50.068	200
mix2-cooler	30	200
biodiesel layer	30	200
bio heat	150	190
vap-methanol	150	190
biodiesel hr	150	190
Hot-mixture	200	0.1
ecisonal	200	0.1
pure biodiesel	200	0.1
preheated feed	100	200
cool ecisonal	100.77	0.1
feed hotter	130	190
little meth	100.77	0.1
pure ec	100.77	0.1
meth partially cooled2	82.513	190
more methanol	82.3	190
waste water	50	190
All methanol	83.22	0.1

3. Result and discussion:

3.1 Experimental laboratory results:

The experimental investigation of Jojoba oil transesterification was successfully executed under the conditions that detailed in the methodology (150 ml oil, 6:1 methanol ratio, 50°C, and 30 min). The experimental biodiesel yield was 72 ± 1.41 ml.

Based on the initial volume of raw Jojoba oil (150 ml), the experimental volumetric yield was calculated to be 48%. The theoretical maximum conversion limit for Jojoba wax esters is approximately 52.6% due to the specific stoichiometry that produces both methyl esters and fatty alcohols. Therefore, the experimental yield of

48% represents a reaction efficiency of 91.3% relative to the maximum theoretical limit. This high conversion efficiency confirms that the selected experimental parameters and the sodium carbonate catalyst were highly effective in driving the transesterification reaction forward.

Regarding the visual appearance, the final produced biodiesel, as shown in Figure 4 exhibited a distinct milky white, cloudy appearance.



Fig 4. Jojoba biodiesel.

This non-standard visual characteristic is highly significant and provides crucial chemical insights. The whitish color is not an indication of a failed reaction, but rather confirms the presence of Eicosanol (fatty alcohol). As previously highlighted, Jojoba oil's unique structure results in the production of these long-chain fatty alcohols as byproducts. Since Eicosanol is a waxy substance with a white color and a high melting point, its partial solidification at room temperature is responsible for the cloudy, milky appearance of the crude biodiesel. Additionally, a minor contribution to the cloudy appearance may be attributed to the formation of stable emulsions during the water-washing stage, which trapped small amounts of water and soap.

While the reaction efficiency was high, the experimental phase revealed significant practical limitations, particularly in the downstream separation and purification stages. This directly addresses the difficulties outlined in the methodology chapter and reinforces the necessity of the simulation study.

The primary experimental challenge was the physical separation of the biodiesel from the white, waxy fatty alcohol phase. Standard gravity settling was insufficient for complete phase separation due to the similar densities and the waxy nature of the byproduct. Furthermore, the mandatory water-washing stage led to the formation of persistent emulsions, making it extremely difficult to recover the purified product and causing unavoidable handling losses of the valuable biodiesel. These mechanical losses and separation inefficiencies are the primary reasons why the experimental yield (48%) remained slightly below the maximum theoretical value (52.6%).

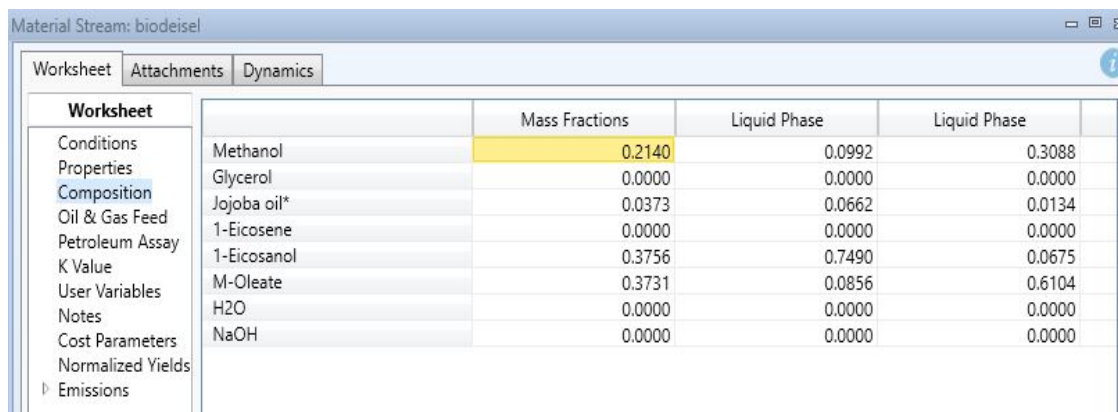
These persistent experimental hurdles regarding phase separation and purity confirmed that conventional lab-scale methods are inadequate for processing Jojoba oil efficiently. Therefore, this phase strongly justified the transition to simulation in Aspen HYSYS, where advanced, industrial-scale separation techniques, such as short-path distillation, could be modeled to overcome these practical limitations.

3.2 Simulation results:

The conversion reactor serves as the primary stage for the transesterification of Jojoba oil. In this simulation, the calibrated Jojoba hypothetical component (563 g/mol) was reacted with methanol at a precise 6:1 molar ratio.

The steady-state simulation of the conversion reactor (CRV-100) indicates a robust and thermodynamically stable process. This is characterized by a perfect mass balance closure, where the total inlet and outlet mass flow rates are maintained at 1.080×10^4 kg/h. Operating at a regulated pressure of 200 kPa ensures that the vapor fraction of the resulting mixture remains at zero, confirming that the reactants are entirely in the liquid phase throughout the process. Furthermore, thermal analysis reveals a distinct exothermic behavior, evidenced by a calculated heat flow duty of -1.170×10^6 kJ/h. This energy release necessitates active thermal management to maintain the isothermal profile observed in the simulation, where the temperature stabilizes exactly at 50 °C.

The chemical composition of the reactor effluent confirms the successful transesterification of Jojoba oil into methyl esters (specifically modeled as M-Oleate), as illustrated in Figure 5.



The screenshot shows the 'Material Stream: biodeisel' window in Aspen HYSYS. The 'Worksheet' tab is active, displaying a table of mass fractions for various components. The components are listed in the first column, and their mass fractions are shown in the subsequent columns. The components are: Methanol, Glycerol, Jojoba oil*, 1-Eicosene, 1-Eicosanol, M-Oleate, H2O, and NaOH. The mass fractions are: Methanol (0.2140), Glycerol (0.0000), Jojoba oil* (0.0373), 1-Eicosene (0.0000), 1-Eicosanol (0.3756), M-Oleate (0.3731), H2O (0.0000), and NaOH (0.0000). The table also includes columns for 'Liquid Phase' and 'Liquid Phase'.

	Mass Fractions	Liquid Phase	Liquid Phase
Methanol	0.2140	0.0992	0.3088
Glycerol	0.0000	0.0000	0.0000
Jojoba oil*	0.0373	0.0662	0.0134
1-Eicosene	0.0000	0.0000	0.0000
1-Eicosanol	0.3756	0.7490	0.0675
M-Oleate	0.3731	0.0856	0.6104
H2O	0.0000	0.0000	0.0000
NaOH	0.0000	0.0000	0.0000

Fig 5. Mass fraction composition of the biodiesel stream exiting the conversion reactor.

The results show an M-Oleate mass fraction of 0.3731. A defining characteristic of this reaction is the nearly equal mass fraction of 1-Eicosanol (0.3756), the primary fatty alcohol byproduct generated when Jojoba wax esters are cleaved. This validates the unique chemical behavior of Jojoba oil, which produces high value alcohols instead of glycerol (recorded as 0.0000 mass fraction). The presence of unreacted Jojoba oil (0.0373) confirms highly efficient conversion while justifying the 95% conversion assumption used in the model. Additionally, the excess methanol fraction (0.2140) confirms that the 6:1 molar ratio provides a significant surplus to drive the reaction forward, necessitating downstream recovery.

The purification efficacy of the combined water-washing and decanting stage is clearly demonstrated when comparing the crude reactor effluent to the refined intermediate stream. In the initial crude stream, methanol was present at a high mass fraction of 0.2140. Following the integration of the washing unit and gravity-based separation in Aspen HYSYS, the molar composition of the refined stream shows that the methanol concentration was successfully reduced to a mole fraction of 0.0921 as shown in figure 6.

Material Stream: biodiesel hr

Worksheet		Mole Fractions	Vapour Phase	Liquid Phase
Conditions	Methanol	0.0921	0.6988	0.0622
Properties	Glycerol	0.0000	0.0000	0.0000
Composition	Jojoba oil*	0.0231	0.0000	0.0296
Oil & Gas Feed	1-Eicosene	0.0000	0.0000	0.0000
Petroleum Assay	1-Eicosanol	0.4396	0.0001	0.6928
K Value	M-Oleate	0.4400	0.0000	0.2121
User Variables	H2O	0.0052	0.3010	0.0033
Notes	NaOH	0.0000	0.0000	0.0000
Cost Parameters				
Normalized Yields				
Emissions				

Fig 6. Molar composition of the biodiesel stream following water washing and gravity separation.

As a direct result of this solvent removal, the product stream became significantly more concentrated with the primary target components with mole fractions of M-Oleate and 1-Eicosanol shifted to 0.4400 and 0.4396, respectively, making them the dominant species entering the final purification stage.

To ensure the reliability and predictive accuracy of the Aspen HYSYS model, a validation step was conducted by comparing the simulation outputs with the experimental compositional analysis of the biodiesel mixture prior to the SPD stage. The fuel's molecular profile is dominated by the C21-C25 fraction, comprising both the target methyl esters and heavy fatty alcohol byproducts (e.g., 1-Eicosanol). Experimental analysis indicated that this fraction constitutes 46% of the mixture, while the HYSYS model predicted 43% as shown in Figure 6(a percentage error of approximately 6.5%). The close agreement between these values confirms the model's effectiveness in capturing the complex nature of the Jojoba oil transesterification products. These heavy fractions (C21-C25) are known to induce persistent emulsions, rendering gravity settling ineffective and validating the necessity of the thermal separation approach implemented in this study.

The final and most critical refinement stage involves the thermal separation of the methyl esters from the heavier fatty alcohols utilizing a Short Path Distillation (SPD) unit. As depicted in Figure 7, the molar composition of the final "pure biodiesel" stream demonstrates a remarkable enhancement in product quality.

Material Stream: pure biodiesel

Worksheet		Mole Fractions	Vapour Phase	Liquid Phase
Conditions	Methanol	0.0000	0.1684	0.0000
Properties	Glycerol	0.0000	0.0000	0.0000
Composition	Jojoba oil*	0.0032	0.0396	0.0032
Oil & Gas Feed	1-Eicosene	0.0000	0.0000	0.0000
Petroleum Assay	1-Eicosanol	0.0251	0.7825	0.0251
K Value	M-Oleate	0.9717	0.0000	0.9717
User Variables	H2O	0.0000	0.0095	0.0000
Notes	NaOH	0.0000	0.0000	0.0000
Cost Parameters				
Normalized Yields				
Emissions				

Fig 7. Molar composition of the highly purified biodiesel stream exiting the SPD unit.

When compared to the intermediate stream, the distillation process achieved complete elimination of residual volatile solvents, reducing both methanol and water mole fractions to an absolute 0.0000. More significantly, the SPD unit successfully fractured the challenging biodiesel-alcohol mixture; the mole fraction of the primary byproduct, 1-Eicosanol, was drastically reduced from 0.4396 down to a mere 0.0251.

The overall plant performance was evaluated through mass yield and resource recovery. The steady-state data shows that a Jojoba oil feed of 8,051.06 kg/h resulted in a final "pure biodiesel" output of 4,158 kg/h. This equates to an actual process yield of approximately 51.64%, representing 98.2% of the theoretical maximum yield. Furthermore, the simulation managed an initial methanol load of 2,745.99 kg/h and successfully isolated 2,284 kg/h in the "Recovery Methanol" stream, achieving an excellent recovery rate of 83.1%.

To evaluate the fuel quality under international testing standards (40 °C and 101.3 kPa), the physical properties of the produced biodiesel were reassessed. At 40 °C, the mass density was determined to be 857.6 kg/m³, placing it well within the acceptable range for commercial biodiesel. The simulation recorded a kinematic viscosity of 7.758 cSt. Although this value slightly exceeds the ASTM D6751 upper limit of 6.0 cSt, this is a scientifically expected result. This elevation is not a process failure but is naturally caused by the unique chemical composition of Jojoba oil, which is characterized by longer carbon chains (such as Eicosenoic acid, C20:1) and the presence of heavy fatty alcohols, in contrast to standard triglyceride-based vegetable oils. Using this fuel directly in standard diesel engines without modification could potentially lead to operational issues, such as poor atomization, incomplete combustion, and increased deposit formation within the fuel system.

To mitigate these limitations, fuel blending strategies are highly recommended. As highlighted by Mustayen et al. (2022), blending high-viscosity biofuels with conventional diesel is a practical and effective methodology to optimize fuel properties, reduce viscosity, and ensure compliance with regulatory standards for commercial engine application.

4. Conclusions:

This study successfully addressed the critical physical separation bottlenecks inherent in biodiesel production from crude Jojoba oil. While laboratory experiments demonstrated high chemical conversion using a base-catalyzed single-step transesterification, the subsequent formation of severe waxy emulsions driven by the generation of heavy fatty alcohols like 1-Eicosanol rendered traditional gravity decanting highly inefficient. To overcome this industrial barrier, a rigorous continuous process simulation was developed using Aspen HYSYS, providing a highly scalable thermal separation framework. Based on the integrated experimental and computational analyses, the following key conclusions can be drawn:

1. **Thermodynamic Modeling and Simulation Accuracy:** To overcome the physical limitations observed in the laboratory, Jojoba oil was meticulously defined in Aspen HYSYS as a hypothetical component with a calibrated molecular weight of 563 g/mol. Coupled with the NRTL fluid package, this thermodynamic model successfully simulated the complex phase behavior of the waxy emulsions, providing a reliable digital framework to design and test the thermal separation process without the need for extensive experimental trials..
2. **Resolution of the Separation Bottleneck:** The implementation of a Short Path Distillation (SPD) unit operating under an extreme vacuum of 0.1 kPa proved exceptionally effective. The thermal separation successfully fractured the biodiesel-alcohol mixture without causing thermal degradation, yielding a high-purity methyl ester stream (97.17%) and virtually eliminating the residual waxy byproducts.
3. **Process Economics and Efficiency:** The steady-state simulation demonstrated robust industrial viability, achieving an actual process mass yield of 51.64%, which represents an impressive 98.2% of

the theoretical maximum. Furthermore, the designed multi-stage purification train successfully recovered 83.1% of the unreacted methanol, significantly reducing projected operational costs.

4. **Fuel Quality Compliance:** The synthesized Jojoba biodiesel demonstrated a density of 857.6 kg/m³, well within commercial standards. While the kinematic viscosity (7.758 cSt) slightly exceeds the ASTM D6751 upper limit of 6.0 cSt, this is a chemically expected outcome due to the oil's inherent long-chain wax esters. To optimize fuel properties and ensure full regulatory compliance for commercial engine applications, blending this biodiesel with conventional diesel is recommended as a practical and effective strategy.

Ultimately, this research validates that integrating advanced thermal separation technologies like SPD with precision simulation tools provides a highly viable, sustainable, and scalable pathway for commercializing non-edible, arid-land feedstocks for green energy production.

Author Contributions

Dr. Muna conducted the laboratory experiments. Abraheem Jirhiman and Dr. Tarek Hamad were responsible for the conceptualization, simulation model development, and manuscript writing.

Conflict of Interest

The authors' declaration of interest is as follows: "None declared".

Data Availability

The data that support the findings of this study are available from the corresponding author upon request.

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