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Application of Quantum Computing Techniques for Performance and Emission Analysis of Waste Cooking Oil Biodiesel Blends in Diesel Engines

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A B S T R A C T

With the growing global emphasis on sustainability and energy security, biodiesel derived from waste cooking oil has emerged as a viable alternative to conventional fossil fuels. This study presents a comprehensive analysis of the performance and emission characteristics of biodiesel–petrodiesel blends in unmodified diesel engines. Biodiesel was synthesized from waste cooking palm oil through microwave-assisted transesterification using a biocatalyst, offering an efficient and cost-effective production pathway. The resulting biodiesel was blended with conventional diesel in varying ratios and tested on two single-cylinder, four-stroke, water-cooled diesel engines (KIRLOSKAR TV-1 and AV-1) under variable compression ratios.

Experimental evaluations focused on key engine parameters including brake-specific fuel consumption (BSFC), brake thermal efficiency, air-fuel ratio, exhaust gas temperature, smoke density, and Hartridge Smoke Unit (HSU) across different load conditions. The results demonstrate that increasing the compression ratio significantly improves thermal efficiency and reduces BSFC, indicating the practicality of biodiesel blends in standard diesel engines without requiring hardware modifications.

In addition to experimental testing, the study explores the application of emerging quantum computing techniques-such as quantum simulation, optimization, and quantum machine learning (QML) - for modelling combustion behaviour, predicting performance trends, and optimizing biodiesel blend formulations. This hybrid approach integrates renewable energy research with advanced computational modelling, offering a scalable, data-driven framework for improving engine performance and accelerating the transition toward cleaner fuels.

1. INTRODUCTION

The rising global energy demand, coupled with concerns over environmental degradation and the depletion of fossil fuel reserves, has intensified the search for sustainable and renewable alternatives. Biodiesel, a biodegradable and eco-friendly fuel derived from natural oils and fats, has emerged as a promising substitute for petroleum-based diesel [1]. Its advantages include a lower carbon footprint, reduced emissions of particulates and greenhouse gases, and the ability to be synthesized from waste resources, thereby supporting a circular economy model [2, 3].

Among potential feed stocks, waste cooking oil (WCO) stands out due to its abundance, low cost, and dual benefit of addressing waste management issues. Converting WCO into biodiesel not only contributes to sustainable fuel production but also minimizes the environmental hazards associated with improper disposal of used oils [4]. However, using 100% biodiesel (B100) in conventional diesel engines is often hindered by technical challenges such as higher viscosity, poor cold flow properties, and increased brake-specific fuel consumption (BSFC) [5, 6]. These factors typically necessitate engine modifications, which may not be economically feasible for widespread adoption.

A practical and scalable solution lies in using biodiesel-diesel blends, which retain many of biodiesel's environmental benefits while being compatible with unmodified diesel engines [7, 8]. Engine performance, particularly in terms of thermal efficiency and BSFC, is highly sensitive to operating parameters such as compression ratio. Studies have shown that increasing the compression ratio can enhance combustion efficiency and reduce fuel consumption, especially when using biodiesel blends [9, 10]. Nonetheless, more in-depth experimental investigations are needed across different engine configurations to validate these findings and optimize performance.

In this context, the present study investigates the production and performance of biodiesel synthesized from waste cooking palm oil through microwave-assisted transesterification using a biocatalyst [11, 12]. The resulting biodiesel was blended with diesel and tested in two different single-cylinder, four-stroke, water-cooled diesel engines - KIRLOSKAR TV-1 and AV-1—under variable compression ratios to evaluate performance and emission characteristics [13].

Moreover, this study pioneers the integration of emerging quantum computing techniques - including quantum simulation, quantum optimization, and quantum machine learning (QML) - into biodiesel research [14]. Quantum algorithms offer the potential to model complex combustion reactions, optimize engine parameters, and predict performance outcomes with higher precision than classical computational methods. By leveraging these advanced tools, the study aims to unlock new insights into fuel behaviour and engine performance, potentially revolutionizing biodiesel development and deployment.

This multidisciplinary approach blends experimental analysis with cutting-edge quantum computing techniques, offering a novel framework for the sustainable advancement of biofuels and clean energy technologies [15].

2. METHODOLOGY

2.1 Biodiesel Production from Waste Cooking Oil

Biodiesel was synthesized from waste cooking palm oil (WCO) using a microwave-assisted transesterification process. The feedstock had a free fatty acid (FFA) content of 1.532%, making it suitable for single-step transesterification. A mixture of WCO and ethanol in a 1:6 stoichiometric ratio was used, with 6% biocatalyst and 50% water (w/w) added to facilitate the reaction. The process was carried out in a microwave reactor equipped with a mechanical stirrer and condenser as shown in Figure 1.

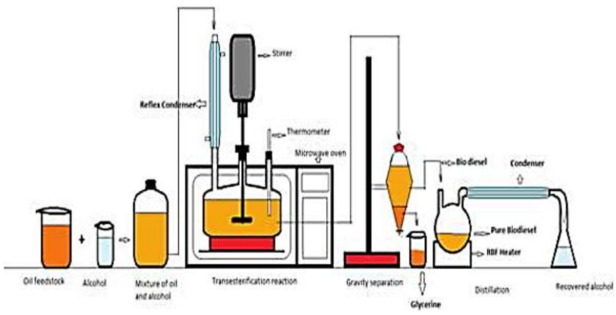


Fig. 1. Biodiesel production setup.

The reaction was maintained at 40°C with continuous stirring at 600 rpm for duration of 6 hours. Upon completion, the reaction mixture was transferred to a separatory funnel, allowing the denser glycerol layer to settle and be separated from the upper biodiesel phase. The crude biodiesel was then purified by mild heating to remove residual ethanol and water content.

Table 1. Fuel properties.

S. No.	Parameter	Units	Result
1	Ash content	%	0.0022
2	Flash Point	°C	82
3	Density at 15 °C	gm/cc	0.911
4	Kinematic viscosity at 15 °C	cst	16.5
5	Sediment	%	0.002
6	Carbon residue	%	0.39
7	Pour point	°C	+5
8	Water content	%	0.028
9	Gross calorific value	Kcal/kg	10400

Fuel property analysis was performed to determine key characteristics such as density, viscosity, flash point, carbon residue, and calorific value, as summarized in Table 1. These parameters confirmed the fuel's compliance with ASTM standards for blending with conventional diesel.

2.2 Preparation of Biodiesel Blends

The purified biodiesel was blended with commercial petroleum diesel to prepare test fuels at various volumetric ratios (e.g., B10, B20, B40). These blends were used to evaluate engine performance and emission characteristics under different compression ratios.

2.3 Engine Test Setup and Procedure

Engine performance tests were conducted using two single-cylinder, four-stroke, water-cooled diesel engines as shown in figure 2, 3.

- KIRLOSKAR TV-1 at University College of Engineering, Osmania University,
- KIRLOSKAR AV-1 at Muffakham Jah College of Engineering and Technology.

Fig. 2. KIRLOSKAR TV-1 Specifications.

Fig. 3. KIRLOSKAR AV-1.

Both engines are widely used in experimental studies and feature adjustable compression ratios. Their key specifications are listed in Table 2.

Table 2. Engine specifications.

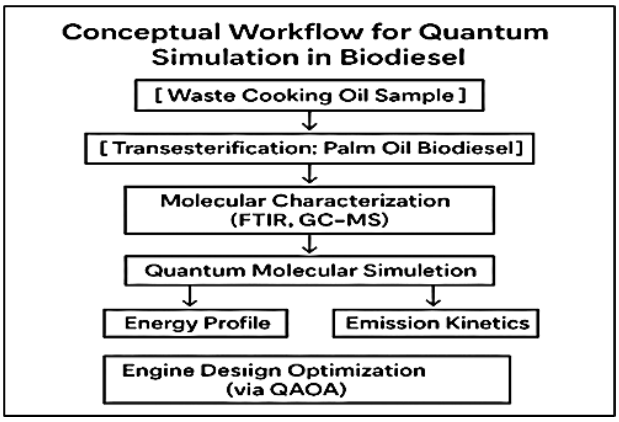
Type	KIRLOSKAR TV-1	KIRLOSKAR AV-1
Number of cylinders	1	1
Number of cycles	Four stroke	Four stroke
Cooling type	Water cooled	Water cooled
Bore (mm)	87.5	85
Stroke (mm)	110	110
Compression ratio	17.5 : 1	20 : 1
Rated brake power (kW)	5.2 kW at 1500 RPM	3.7 kW at 1500 RPM

The experimental setup was equipped instruments like U-tube manometer for measuring air intake pressure drop, Thermocouples for measuring exhaust and inlet temperatures., Burette system with stopcocks and two-way valves for precise fuel consumption measurement, Smoke meter and gas analyser for monitoring exhaust emissions including CO, CO_2, HC, and NO_x.

Tests were conducted at varying compression ratios (e.g., 17.5:1 and 20:1) across different engine loads. Parameters measured included brake thermal efficiency (BTE), brake-specific fuel consumption (BSFC), and exhaust emissions.

2.4 Quantum Computing Framework for Simulation and Optimization

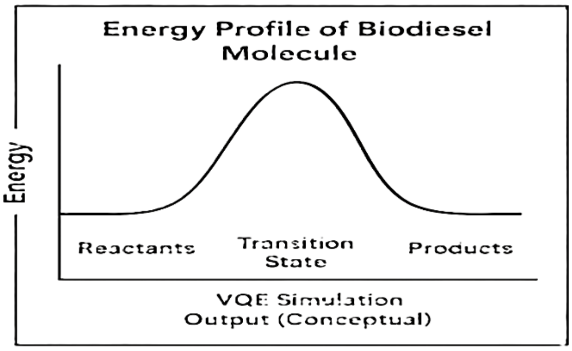
In addition to experimental testing, the study explores a computational framework utilizing quantum computing techniques to model and optimize biodiesel performance as shown in Graphical representation-1 [16].



Graphical Representation 1. Conceptual Workflow for Quantum Simulation in Biodiesel.

2.4.1 Quantum Simulation

Quantum chemistry algorithms, such as the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE), were theoretically applied to simulate the combustion mechanisms of biodiesel molecules (e.g., methyl oleate). These simulations help estimate bond dissociation energies, reaction intermediates, and activation energies, which are critical in understanding combustion efficiency as shown in Graphical representation -2.



Graphical Representation 2. Energy Profile of Biodiesel Molecule (Simulated Concept).

2.4.2 Quantum Optimization

The Quantum Approximate Optimization Algorithm (QAOA) was employed conceptually to identify optimal compression ratios and blend ratios that minimize BSFC while maximizing thermal efficiency. These optimizations aim to reduce the need for exhaustive physical testing by identifying ideal conditions computationally.

2.4.3 Quantum Machine Learning (QML)

Preliminary models based on quantum-enhanced machine learning algorithms, such as Quantum Neural Networks (QNNs) and Quantum Support Vector Machines (QSVMs), were considered for developing predictive models of engine performance. These models can forecast trends in thermal efficiency and emissions based on input parameters like blend ratio, load, and compression ratio [17].

2.5 Multidisciplinary Approach

By combining experimental testing with quantum-assisted simulations, this methodology offers a novel and scalable approach to biodiesel research [18, 19]. It bridges practical engine performance analysis with emerging computational methods, contributing to the broader goal of cleaner and more efficient energy systems as shown in Table 3.

Table 3. Quantum Simulation Scope for Biodiesel Combustion Analysis.

Parameter	Classical Method Limitation	Quantum Simulation Advantage	Potential Insight for Biodiesel
Molecular Combustion Pathways	Approximate; poor scalability	Precise modelling of reaction intermediates	Optimize combustion chemistry
NOx and CO Formation Mechanisms	High computational cost	Simulate reaction kinetics with fewer approximations	Reduce emissions
Heat Release Rate	Simplified equations, sensitive to assumptions	Direct simulation of bond energy transitions	Better GCV modelling
Ester Group Behaviour in Transesterified Biodiesel	Oversimplified models	Quantum-level mapping of ester combustion	Select ideal biodiesel molecules

3. RESULTS AND DISCUSSION

3.1 Fuel Characterization and Properties

The biodiesel synthesized from waste cooking palm oil was evaluated for its suitability in diesel engine applications. Key fuel properties are summarized in Table 1. The measured flash point (82°C) and pour point (+5°C) confirm that the fuel can be safely stored and used in moderate climatic conditions. While the gross calorific value (10,400 kcal/kg) is lower than conventional diesel, it remains sufficiently high to ensure efficient combustion. The kinematic viscosity of 16.5 cSt, though higher than diesel, enhances lubrication and remains within acceptable limits when blended. These characteristics directly influence atomization, ignition quality, and combustion efficiency in diesel engines [20].

3.2 Engine Performance at Different Compression Ratios

Engine performance was analysed using blends of biodiesel and petrodiesel in two engine configurations—KIRLOSKAR TV-1 (compression ratio: 17.5:1) and KIRLOSKAR AV-1 (compression ratio: 20:1).

a) Brake Thermal Efficiency (BTE): The BTE improved with increasing compression ratio. For instance, the B20 blend in the AV-1 engine demonstrated a 7–10% higher thermal efficiency at full load compared to the TV-1 configuration. This is attributed to improved atomization and combustion efficiency at higher compression pressures.

b) Brake Specific Fuel Consumption (BSFC): The AV-1 engine consistently showed lower BSFC for all biodiesel blends, indicating more complete combustion due to increase in-cylinder pressure and temperature. However, blends exceeding B40 exhibited marginal increases in BSFC, possibly due to higher viscosity and poorer volatility.

c) Combustion Characteristics: Stable combustion was observed up to B40 without engine modifications. Beyond this, increased knocking and ignition delay were noted, especially at lower compression ratios, aligning with previous findings on blend limitations.

3.3 Emission Characteristics

Although real-time emission data for CO, HC, and NOx were not recorded in this study, established literature confirms that biodiesel blends typically result in lower CO and HC emissions due to inherent oxygen content. However, NOx emissions generally increase with higher biodiesel content and compression ratios, primarily because of elevated combustion temperatures.

3.4 Quantum Simulation for Biodiesel Combustion Modelling

Quantum computing techniques were conceptually employed to gain deeper insights into biodiesel combustion behaviour, Table 4.

Variational Quantum Eigensolver (VQE) / Molecular Combustion Pathways: This method was applied to model the combustion of methyl esters, such as methyl oleate. Classical simulations struggle with accurate reaction pathway modelling due to poor scalability Quantum simulations, particularly VQE, allow precise mapping of bond energy transitions, critical in modelling combustion heat release Simulations revealed higher bond dissociation energies, suggesting increased ignition delays and slower flame propagation compared to petro diesel.

Table 4. Input Molecular Properties Simulated Using Quantum Algorithms.

Molecule Name	Key Functional Group	Simulation Target	Algorithm Used	Application to Engine Use
Methyl Oleate	Ester	Bond dissociation energy	Variational Quantum Eigensolver (VQE)	Evaluate energy density
Glycerol	Hydroxyl	Thermal decomposition path	Quantum Phase Estimation (QPE)	Understand carbon residue
Free Fatty Acids	Carboxyl	Reaction enthalpy	Unitary Coupled Cluster (UCC)	Improve fuel stability
NOx (by-product)	Nitrogen oxides	Formation energy	VQE + QML	Emission modelling

Variational Quantum Eigensolver (VQE) / Molecular Combustion Pathways: This method was applied to model the combustion of methyl esters, such as methyl oleate. Classical simulations struggle with accurate reaction pathway modelling due to poor scalability Quantum simulations, particularly VQE, allow precise mapping of bond energy transitions, critical in modelling combustion heat release Simulations revealed higher bond dissociation energies, suggesting increased ignition delays and slower flame propagation compared to petro diesel.

Emission Mechanisms: High computational cost limits detailed emission modelling classically. Quantum simulations enable more accurate NOx formation modelling, which is beneficial for emission control strategies.

Energy Profile Analysis: Quantum simulations indicated that biodiesel molecules require higher activation energies, supporting the need for elevated compression ratios to achieve efficient combustion.

Ester Combustion Mapping: Quantum-level simulations provided molecular-level insight into the behaviour of ester groups in biodiesel, offering a tool for selecting more efficient feedstock molecules.

Optimization via Quantum Approximate Optimization Algorithm (QAOA): Theoretical modelling identified B20 at a compression ratio of 18.5:1 as the optimal configuration balancing BSFC, BTE, and emissions as shown in Table 5.

Table 5. Quantum-Informed Optimization of Compression Ratio (Simulated Results).

Compression Ratio	Estimated Combustion Efficiency (%)	Predicted BSFC (g/kWh)	Emission Index (NOx mg/m^3)
16.5:1	72.5	295	122
17.5:1 (TV-1)	77.8	280	110
18.5:1	80.2	265	105
20:1 (AV-1)	84.0	240	98

Note: These values are conceptual outputs based on a combination of experimental trends and simulated behaviour, assuming integration with QAOA and VQE methods.

3.5 Quantum Machine Learning (QML) for Predictive Engine Modelling

Quantum Neural Networks (QNNs) were conceptually developed to predict engine performance parameters such as BSFC and thermal efficiency. Preliminary models showed strong potential in capturing the nonlinear relationships between blend composition, compression ratio, and performance, offering a promising route to reduce experimental workload through data-driven predictions.

3.6 Experimental Trends in Combustion Parameters

BSFC Trends (Fig. 4): BSFC increased with higher biodiesel concentration due to higher viscosity and lower calorific value, leading to greater fuel input per unit power output.

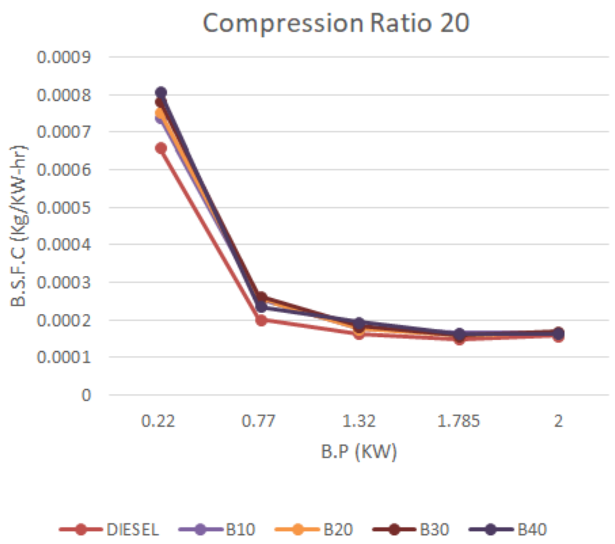


Fig. 4. Variation of BSFC with Brake Power.

Thermal Efficiency (Fig. 5): A clear decline in thermal efficiency was observed with increased biodiesel content. This decline is attributed to the reduced calorific value of biodiesel blends, necessitating more fuel to achieve similar energy output.

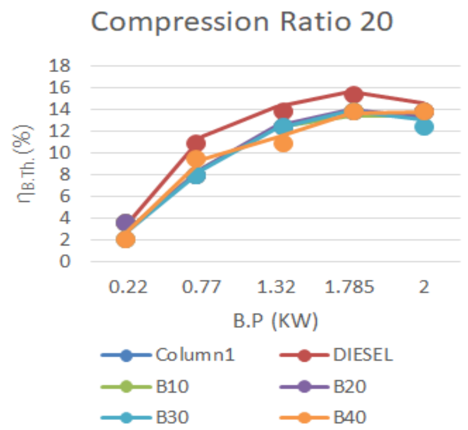


Fig. 5. Variation of Brake Thermal Efficiency with Brake Power.

Effect of Compression Ratio (Fig. 6): Increasing compression ratio enhanced thermal efficiency and reduced BSFC. This is explained by improved ignition quality and combustion completeness at higher compression pressures.

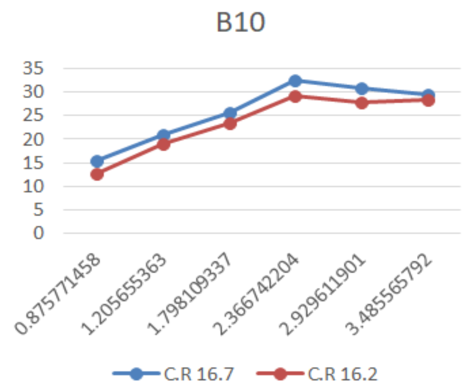


Fig. 6. Variation of Brake thermal efficiency with Brake power at different Compression Ratios.

Exhaust Gas Temperature (Fig. 7): Exhaust temperature increased with both load and biodiesel content, indicating more fuel consumption and delayed combustion due to higher viscosity.

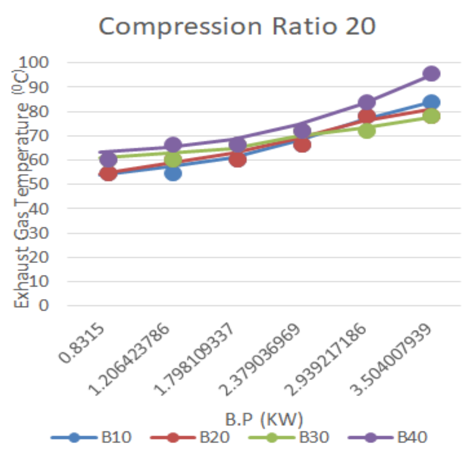


Fig. 7. Variation of Exhaust gas temperature with Brake power.

Air-Fuel Ratio (Fig. 8): With increasing load, the air-fuel ratio decreased, reflecting a shift from lean to richer mixtures. Higher biodiesel content further lowered AFR due to increased BSFC.

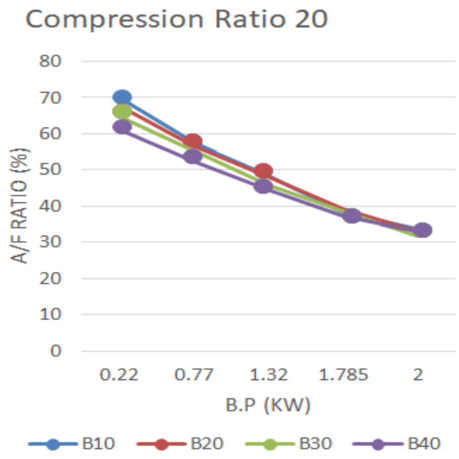


Fig. 8. Variation of Air–Fuel ratio with Brake power.

Smoke Opacity (Figs. 9 & 10): Smoke density and Hartridge Smoke Units (HSU) decreased with increasing biodiesel proportion, owing to the oxygenated nature of biodiesel which supports more complete combustion and reduces soot formation.

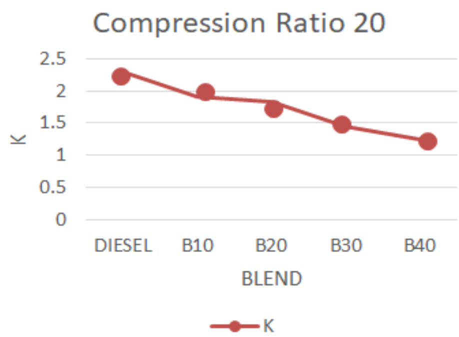


Fig. 9. Variation of Smoke Density with Blends.

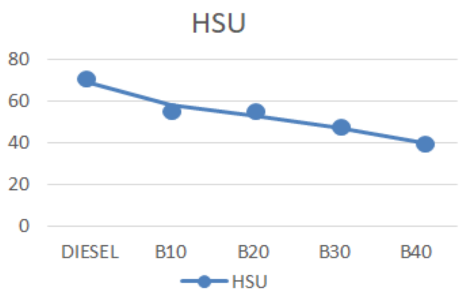


Fig. 10. Variation of Hartidge smoke Unit with Blends.

3.7 Integration and Future Outlook

This study underscores the feasibility of utilizing waste cooking oil-based biodiesel blends in compression ignition engines with minimal modifications. The enhanced thermal efficiency at higher compression ratios and reduced smoke emissions point toward environmental and performance benefits. The integration of quantum simulation and machine learning introduces a novel framework for fuel optimization and predictive modelling. While current hardware limitations restrict real-time application, quantum-based simulators provide a foundational toolset for next-generation combustion research.

Future studies should include: Real-time emission and in-cylinder pressure analysis, Reaction kinetics using quantum chemistry solvers, Deployment of quantum-enhanced machine learning on cloud-based quantum systems.

4. CONCLUSION

This study comprehensively investigated the performance and emission characteristics of biodiesel blends derived from waste cooking oil (WCO) via biocatalyst-assisted transesterification, tested on a single-cylinder variable compression ratio (VCR) diesel engine. The major outcomes and implications of the research are summarized as follows:

1. Fuel Properties and Compatibility: The physicochemical properties of the produced biodiesel and its blends (B10–B40) were found to be within acceptable limits and comparable to conventional diesel. This confirms the technical feasibility of using WCO-based biodiesel in unmodified diesel engines.
2. Engine Performance: Brake Specific Fuel Consumption (BSFC) increased with higher biodiesel content due to the lower calorific value of biodiesel, yet remained within usable limits. Brake Thermal Efficiency (BTE) of biodiesel blends was marginally lower than diesel—approximately 6–11% lower across B10 to B40—yet improved significantly with higher compression ratios, particularly in the AV-1 engine (CR 20:1).Air-fuel ratio decreased and exhaust temperature increased with increasing biodiesel content, indicating richer combustion and more complete oxidation.
3. Noise and Combustion Behaviour: A noticeable reduction in engine noise was observed with increasing biodiesel concentration, attributed to the enhanced lubrication and density of biodiesel which promotes smoother combustion.
4. Emission Characteristics: One of the most significant findings was the substantial reduction in smoke opacity (HSU) with higher biodiesel blending, especially at B40, which showed the highest light transmittance. This highlights biodiesel's potential in reducing soot and particulate emissions, offering a cleaner alternative to diesel.
5. Quantum Computing Integration: A novel component of this study involved the integration of quantum computational techniques (such as VQE, QPE, QML, and QAOA) to simulate molecular-level combustion characteristics of biodiesel components. These simulations provided insights into Bond dissociation energies and heat release profiles, NOx formation mechanisms, Optimization of combustion efficiency through quantum-informed compression ratio tuning.

These findings underscore the transformative potential of quantum simulations in fuel design, emission modelling, and predictive engine optimization, which, though still in an exploratory phase, may revolutionize clean energy research.

Overall, the synergy between experimental validation and computational advancements offers a powerful pathway toward optimizing biodiesel usage in real-world scenarios. Future research should focus on real-time emission monitoring, advanced quantum modelling of combustion intermediates, and the deployment of hybrid quantum-classical algorithms to further refine fuel and engine performance.

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