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Numerical investigation of combustion characteristics of extended coherent flame model 3 zones (ECFM-3Z) in diesel engines running with biodiesel

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Abstract

This research investigates the application of Extended Coherent Flame Model-3 Zones (ECFM-3Z) to assess the performance and emissions of rapeseed oil methyl ester (ROME). Experimental tests were carried out using a Lombardini 3 LD 350 model single-cylinder diesel engine, at 1600-3000 rpm with 200 rpm speed increments, under full load conditions. For numerical analysis, STAR-CD/ESICE software was employed. Methyl Oleate (C₁₉H₃₆O₂) was predicted as the surrogate biodiesel based on Gas Chromatography (GC) analysis and average mass calculation. Notably, the numerical analysis revealed a remarkable similarity in brake power between the experimental and computational investigations. In the range of 2400-3000 rpm, the biodiesel's performance exhibited a maximum deviation of 5%, primarily attributed to pumping, thermal, and friction losses. In terms of emissions, carbon dioxide (CO₂) emissions were consistent with the findings of the experimental study, with a maximum disparity of 10%. However, carbon monoxide (CO) emissions ranged from 57% to 65% lower than those observed in the experimental study, while nitrogen oxide (NO_x) emissions exhibited a reduction of 63% to 84%. In contrast, oxygen (O₂) emissions were notably higher, ranging from 93% to 117% compared to the experimental study, and exhaust temperatures were elevated by 33% to 49% in comparison to the experimental results.

KEYWORDS

3D combustion modeling, alternative fuels, biofuels, internal combustion engines

Abbreviations: ATDC, After Top Dead Center; BTDC, Before Top Dead Center; BDC, Bottom Dead Center; B5, Up to 5% Biodiesel; B10, Up to 10% Biodiesel; B20, 6% to 20% Biodiesel; B100, Pure Biodiesel; CAD, Crank Angle Degree; CFD, Computation Fluid Dynamics; CO, Carbon monoxide; CO $_2$. Carbon dioxide; $C_{19}H_{36}O_2$, Methyl Oleate; ECFM, Extended Coherent Flame Model; ECFM-3Z, Extended Coherent Flame Model-3 Zones; EU, European Union; FAME, Fatty Acid Methyl Esters; GC, Gas Chromatography; GHG, Greenhouse Gases; HV, Heating value; HC, Hydrocarbon; LHV, Latent heat of vaporization; KH-RT, Kelvin-Helmholtz and Rayleigh-Taylor; LHE, Lower Latent Heat of Vaporization; MRC, Marmara Research Center; Mt, Million Tonnes; NaOH, Sodium Hydroxide; NO $_X$, Niltrogen Oxide; RNG, Re-Normalization Group; ROME, Rapeseed Oil Methyl Ester; SO $_X$, Sulfur Oxides; TAB, Taylor Analogy Breakup; TDC, Top Dead Center; TUBITAK, The Scientific and Technological Research Council of Turkey; UHC, Unburned Hydrocarbon; WPOME, Waste Palm Oil Methyl Ester.

1 | INTRODUCTION

The emission of greenhouse gases and the consequential climate change represent a significant global environmental challenge. Transportation sector is one of the key contributors to these emissions, with road transport. Compression ignition engines significantly contribute to the emission of greenhouse gases (GHGs) and other harmful pollutants, posing a severe threat to the environment and human health. Further, these combustion byproducts, such as carbon monoxide (CO), unburned hydrocarbons (UHC), nitrogen oxides (NO_x),

sulfur oxides (SO_x), suspended particulate matter, and aldehydes contribute to respiratory and cardiovascular diseases in humans. Moreover, they play a role in global warming, acid rain formation, and climatic instability.² Using alternative fuels is a measure to reduce harmful emissions. The European Union (EU) wants to increase the share of renewable energy used in transportation to at least 14% by 2030, with a necessary minimum allocation of 3.5% for advanced biofuels.³ The total amount of biofuels consumed as of 2020 was 15.8 million tons (Mt). The distribution of biofuel utilization was as follows: biodiesel constituted 82%, bioethanol accounted for 15%, and biogas contributed 2%.⁴ The utilization of highly oxygenated alcohol-based biofuels presents an effective strategy for reducing these harmful emissions.¹

Biodiesel is defined as fatty acid methyl esters (FAME) produced by reacting short-chain alcohols with various vegetable and animal oils, such as sunflower, olive, cottonseed, rapeseed, safflower, waste frying, and fish oils.⁵ The main concern regarding vegetable oil is its high viscosity, which has a negative effect on engine operation. This viscosity also leads to carbon buildup in the combustion chamber and engine fouling. As a result, researchers are making significant efforts to either chemically alter the vegetable oil or blend it with diesel fuel to prevent engine failure. Of the numerous methods published in the literature, the most effective approach is to chemically transform vegetable oil into a monoalkyl ester of fatty acids, often known as fatty acid methyl ester or ethyl ester, through the process of transesterification.^{2,6,7} Biodiesel fuel shows great promise for the future due to its characteristics comparable to those of diesel fuel. Biodiesel fuels have gained recent attention due to their physical and chemical characteristics, including a higher oxygen content in their chemical structure, higher cetane numbers, increased viscosity and density, lower latent heat of vaporization (LHV), and their derivation from renewable sources. It contains 10%-12% oxygen by mass. 10-12 The utilization of biodiesel leads to decreased CO emissions¹³ and UHC emissions. 2,14,15 But NO_x emissions were increased compared to diesel fuel. 2,10-12,16,17 When compared to diesel fuels, biodiesel fuels have benefits, such as biodegradability, non-toxicity, better lubrication, and lower exhaust pollutants. 18 Biodiesel has flame properties similar to those of diesel fuel, despite having a distinct whirling flame behavior.¹⁹ Biodiesel can be blended with diesel fuel and used in various concentrations. The most common biodiesel blends include 5% biodiesel (referred to as B5, containing up to 5% biodiesel) and 6% to 20% biodiesel (known as B20). Due to excellent solvent and lubricant effect of B100, biodiesel can clean fuel system of vehicles and release deposits results from diesel use. These deposits could lead to clogged filters and it can be needed to replace the filters in the first few tanks. Biodiesel can reduce wear in diesel engines.²⁰

Agarwal and Agarwal conducted a study investigating the use of B100 and conventional diesel fuel in two identical unaltered vehicles. Their aim was to assess component wear, including liners and piston rings, as well as carbon deposit accumulation in common rail direct injection engine-equipped vehicles. The research also aimed to evaluate biodiesel's long-term durability and compatibility with engine components compared to diesel fuel. The experiment involved operating

two identical vehicles for 30,000 kilometers under identical conditions on highways, using B100 and diesel fuel under precisely the same operational circumstances. Following the field trials, the engines were disassembled, and experimental assessments were conducted to evaluate wear and carbon deposits. The analysis revealed the highest wear near the top dead center (TDC) in both engines. Notably, pistonring wear was significantly lower in the biodiesel-fueled vehicle. Additionally, carbon deposits on fuel injectors, inlet and exhaust valves, cylinder head, piston top and sides, inlet and exhaust manifolds, as well as lacquer deposits in the fuel tank, were significantly reduced in the biodiesel-fueled vehicle compared to the diesel-fueled vehicle. Interestingly, distinct white deposits were observed on the piston top of the biodiesel-fueled engine, attributed to residual catalyst from the biodiesel production process. This study demonstrated that using biodiesel in modern common rail diesel vehicles leads to reduced wear on engine components and decreased carbon deposits, indicating its suitability and potential for widespread adoption.²¹

Researchers have focused to numerical simulations using computation fluid dynamics (CFD) tools because experimental studies are often expensive and time-consuming, despite the fact that many experimental investigations have examined the usage of biodiesel in diesel engines.²² Furthermore, numerical simulations are useful for giving better clarity to the events taking place inside the engine cylinder.²³ Cihan, Ö²⁴ conducted experiments using 5%, 10%, and 20% biodiesel blends produced from fig seed oil. The study investigated their impact on various engine parameters such as cylinder pressure, pressure increase rate, net heat release rate, brake-specific fuel consumption, engine torque, and exhaust gas temperature. Additionally, the combustion characteristics were numerically validated using AVL Fire software. WAVE model for spray, the k-zeta-f model for turbulence, and the Coherent Flame Model and ECFM-3Z model for combustion were used for the study. The findings showed that up to 10% biodiesel (B10) had better combustion properties compared to conventional fuels. The consistency between numerical and experimental findings demonstrated the reliability of the numerical model. Different spray breakup models, such as Kelvin-Helmholtz-Rayleigh-Taylor (KH-RT), WAVE, CHU, and Taylor Analogy Breakup (TAB), were assessed based on experimental data in research by Ashkezari et al.²⁵ The KH-RT model accurately predicted droplet size resulting from spray fragmentation and penetration. Bishop et al²⁶ conducted a study on numerical modeling of biodiesel blends using the AVL Fire ESED program. They gathered experimental data on engine performance and emissions for four cases, including three B100 cases and one diesel-triacetin case. Combustion and spray dispersion were modeled using the ECFM-3Z and Wave Child Break-up models, while Extended Zeldovich and Lund Flamelet models were used for NO_x and soot emissions. The findings showed that using biodiesel blends in diesel fuel reduced NOx and soot emissions and that the shape of the injection rate was crucial for modeling accuracy. Kolhe et al²⁷ simulated the combustion characteristics of Pongamia Pinnata biodieseldiesel blends using the CFD code FLUENT. Their modeling included sub-models like the droplet collision model and TAB model for spray modeling, and the results demonstrated good agreement with

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experimental data. Manimaran et al 28 investigated the effects of incylinder flow structures, fuel injection, and design parameters on engine performance and emissions using the ECFM-3Z model with ES-ICE and STAR-CD codes. The study revealed that higher NO $_{\rm x}$ emissions occurred at peak temperatures, whereas increased soot and CO emissions were occurred with peak pressures.

While numerous numerical investigations have examined the combustion characteristics of biodiesel fuels derived from diverse feedstocks, the literature is noticeably lacking in comprehensive assessments of how molecular differences in the physical properties of biodiesel affect combustion behavior. Research has specifically shown that viscosity of biodiesel, along with other physical characteristics, can dramatically affect critical factors like spray patterns, fuelair mixing, and ignition. Furthermore, cold flow properties of biodiesel, particularly its viscosity at lower temperatures, have been recognized as critical in determining its atomization and ignition performance under cold conditions. Despite these insights, there exists a substantial gap in the literature for comprehensive analyses of the interactions between these molecular changes in the characteristics of biodiesel and combustion behavior. Moreover, the scarcity of numerical studies that use actual fuel qualities highlights the necessity for indepth research in this field. Addressing this gap could enhance our understanding of biodiesel ECFM-3Z combustion characteristics and contribute to the development of more accurate predictive models for alternative fuel applications.

The statement of novelty in this study is the investigation of the ECFM-3Z approach in terms of performance and emissions of rape-seed oil methyl ester with actual biodiesel specifications. Thus, the initial step in this study was to analyze the biodiesel at the TUBITAK MRC laboratory in compliance with TS EN 14214 standard. The study conducts experimental and numerical analysis of performance and emission characteristics, employing the STAR-CD/ESICE software, and using $C_{19}H_{36}O_2$ as a surrogate biodiesel based on GC analysis and average mass calculation. The investigation is important in this aspect. This comprehensive study seeks to verify the accuracy of the numerical model concerning engine performance and recommends the exploration of alternative spray break-up, atomization, and droplet models for emissions in future investigations.

TABLE 1 The specifications of the Lombardini 3 LD 510.

Bore × Stroke (mm)	85 × 90
Total displacement (cm ³)	510
Compression ratio	17.5:1
Valves/cylinder	2
Power (kW)	8.94
Torque (kg.m)	3.35 at 1800 rpm
Inlet valve opening degree	22 Before Top Dead Center (BTDC)
Inlet valve closing degree	52 After Top Dead Center (ATDC)
Exhaust valve opening degree	46 BTDC
Exhaust valve closing degree	29 ATDC
Injector hole diameter (mm)	0.295

2 | EXPERIMENTAL APPARATUS AND TEST PROCEDURE

The experimental phase of this research was conducted using a Lombardini brand 3 LD 510 model non-road single-cylinder diesel engine, located at the Anadolu Motor Co. Laboratories, a Turkish company. The engine specifications are summarized in Table 1.

The engine was connected to a Barghi & Saveri FE60S eddy current dynamometer and tested within the range of 1600–3000 rpm under full load conditions, using both diesel fuel and B100 biodiesel (Figures 1 and 2). Fuel consumption was determined by measuring the time taken to consume a fixed mass of fuel (50 g).

Despite higher cetane number of biodiesel (Table 2), the static injection timing of 25° BTDC remained constant during all experimental tests. However, in the numerical analysis of biodiesel, injection timing was moved forward by 1 Crank Angle Degree (CAD) compared to diesel fuel based on the experimental results. Additionally, as the engine speed increased, the injection advance for biodiesel was increased by 1°CAD. Injection advance and cetane number are crucial factors for comparing the performance and emission characteristics of internal combustion engines. The cetane number reflects the ability of diesel fuel to self-ignite when injected into the engine cylinders. A lower ignition tendency results in a longer ignition delay time. Increased ignition delay can lead to a higher accumulation of fuel in the combustion chamber. As combustion temperatures rise, $NO_{\rm x}$



FIGURE 1 Experimental test setup.

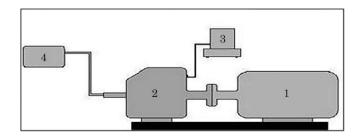


FIGURE 2 Schematic test setup. 1. Dynamometer and control unit 2. Diesel engine 3. Fuel tank 4. Emission analysis equipment.

	3000 rpm	2800 rpm	2600 rpm	2400 rpm
Brake power (kW)	± %0.05	± %0.05	± %0.05	± %0.05
CO ₂ emissions (g/kWh)	±%4.20	±%4.20	±%4.20	±%4.19
CO emissions(g/kWh)	% 4.12	±% 4.10	±%4.08	±%4.17
NO emissions (g/kWh)	±%4.11	±%4.10	±%4.09	±%4.08
O ₂ emissions (g/kWh)	±%4.10	±%4.11	±%4.10	±%4.11
Soot (g/kWh)	±0.01	±0.01	±0.01	±0.01
Exhaust Temperature °K	+%2			

TABLE 2 Relative uncertainties of biodiesel for different engine revolutions.



FIGURE 3 Exhaust emission measurement setup.

emissions increase, and elevated pressures can lead to mechanical stresses and diesel knock.^{29,30} Gaseous emissions were measured using a HORIBA PG-250 emissions analyzer (Figure 3). The relative uncertainties associated with the engine test setup and thermocouples were 0.05% and 2%, respectively.

The engine was fed with fuel from an external tank. Throughout the experiments, a stopwatch was used to time how long it took for 50 grams of fuel to be consumed. Prior to starting data collecting, each test run had a 10-min warm-up time. Measurements included specific fuel consumption, brake power, torque, exhaust emissions and exhaust gas temperatures.

2.1 Uncertainty analysis of engine parameters

The calculation of uncertainty and errors in the experimental data involved taking into consideration of various influencing factors, including the test setup, calibration gases, instrument accuracy, and repeatability.

2.1.1 | Measurement of uncertainty for engine power (set-up) and thermocouple

Certificate error values of test set up and thermocouple were 0.05% and 2% respectively.

2.1.2 | Measurement of uncertainty for exhaust emissions

In order to measure uncertainties of emission gases for different engine revolutions, uncertainties of calibration gases, engine setup and thermocouple were taken into account.

$$\label{eq:uncertainty} \textbf{Uncertainty} = (\text{value}~(X)~*~\%~\text{uncertainty}~\text{in measurement})/100 \end{(2.1)}$$

$$\mathbf{b}(\mathbf{x}) = \text{uncertainty}/\sqrt{1} \tag{2.2}$$

$$\mathbf{b}(\mathbf{x})/\mathbf{X} = \mathbf{b}\mathbf{x}/\mathbf{value} \tag{2.3}$$

Total Uncertainty =
$$\sqrt{\sum (uncertanities)^2}$$
 (2.4)

$$\mathbf{B}(\mathbf{x}) = \text{Total uncertainty} * 7 (O_2 \text{ gas calibrated for } 7\%)$$
 (2.5)

Extended Uncertainty =
$$2^*B(X)$$
 (2.6)

Relative Uncertainty
$$\%$$
 B(x) = (extended uncertainty/7) * 100 (2.7)

Uncertainties of exhaust gases vary according to engine power, engine rpm, temperature of exhaust gases and amount of exhaust gases. Uncertainty calculations for different engine revolutions are given in Table 2.

2.2 | Experimental test fuel and surrogate fuel

The rapeseed oil and Diesel fuel utilized in this investigation were sourced from commercial markets. The selection of the feedstock is crucial in the biodiesel production process. The fatty acid composition of the chosen feedstock notably impacts the physical characteristics of biodiesel. In some countries like Canada, it is known as canola oil, and the leading producer of rapeseed oil produces nearly 19 million tonnes (Mt). Rapeseed oil contains a significant quantity of monounsaturated and polyunsaturated fatty acids, making it an advantageous option for biodiesel production due to their positive effects on fuel stability and quality. Canola seeds have an oil content of 40%–45%. It is one of the best oil plants for energy agriculture because of the high levels of erucic acid and glucosinolate in its oil, which are detrimental

TABLE 3 Specifications of rapeseed oil.

Specifications	Rapeseed Oil
Acid number (mg KOH/g oil)	0.18
Density (g/mL)	0.92
Water content (ppm)	275
lodine number (g iodine/100 g oil)	102
Na (ppm)	2
K (ppm)	11
Mg (ppm)	11
Ca (ppm)	31
P (ppm)	32
Molecular weight (g/mol)	882.8

Note: Analyzed at laboratory of TUBITAK MRC.

to both human and animal health. Oleic acid (56%-64%) and linoleic acid (17%-20%) are the predominant fatty acids in rapeseed oil. 31,32

Because the density difference between canola oil biodiesel and diesel fuel (canola 883.5 kg/m³, diesel fuel 831.5 kg/m³) is less than the viscosity difference (canola 4.32 mm²/s, diesel fuel 2.6 mm²/s), canola biodiesel and diesel fuel mix well.³³ One of the advantages of biodiesel over diesel fuel is its higher oxygen content. Canola biodiesel contains 10%–12% oxygen, which contributes to improved combustion and reduced exhaust emissions (such as particulate matter, carbon monoxide, and hydrocarbons).³⁴

Prior to starting biodiesel production, acid number, water content, metal content, and fatty acid composition of the rapeseed oil was analyzed (Table 3). These parameters are critical factors that influence the effectiveness of the transesterification process. For example, the presence of alkali metals in the oil can result in the formation of soap when they interact with free fatty acids. This soap formation not only diminishes process efficiency but can also negatively impact the quality of the biodiesel if adequate purification is not carried out. Furthermore, free fatty acids and water content in the oil serve as factors that reduce process efficiency.

Biodiesel was produced from rapeseed oil via transesterification reaction at the laboratory of TUBITAK Marmara Research Center (Figure 4). In the production of biodiesel, NaOH functioned as the catalyst while CH₃OH was the alcohol used. During biodiesel production process, various equipments were employed, including a temperature-controlled circulator water bath, heated jacketed reactors of varying capacities (500, 1000, 2500, and 5000 mL), a mechanical mixer, and a cooling system. Methanol-oil ratio was 6:1 and NaOH concentration was maximum 1% relative to the weight of oil. During the experiments, oil was continuously stirred as it was heated in a glass reactor equipped with a heating jacket, gradually reaching a reaction temperature of 65 °C. The transesterification process was initiated by introducing the sodium hydroxide (NaOH) catalyst to the preheated oil at 65 °C, after preheating it to around 40 °C and blending it with methanol. Throughout the reaction, a mechanical stirrer was employed to keep the mixture in the reactor in constant motion, operating at a speed of 700 rpm. After a 2-h reaction period, both the mixing and heating were discontinued to conclude the reaction. The mixture was allowed to stand for 4 h to enable the separation of the biodiesel phase and the glycerol phase within the reactor. The glycerol phase, situated in the lower layer, was drawn out of the reactor via a bottom outlet, effectively isolating the two distinct phases. Excess methanol in the biodiesel was eliminated using a rotary evaporator. The biodiesel was further purified through a washing process, followed by the evaporation of any remaining water using a rotary evaporator to get rid of any remaining catalyst and contaminants.

It is essential to understand the physical characteristics of biodiesel to model processes like spray atomization, droplet breakup, evaporation, and combustion. Biodiesel properties were analyzed in accordance with the TS EN 14214 standard. The properties of both diesel and biodiesel are reported in Table 4.

The fatty acid composition of the biodiesel was determined through GC analysis. This allowed us to establish a surrogate fuel for biodiesel based on the concentrations of fatty acids (Table 5) and average mass calculations (Table 6). A single-component surrogate biodiesel, $C_{19}H_{36}O_2$, was predicted. In the numerical analysis, actual values of density, viscosity, and calorific values were employed.

3 | COMPUTATIONAL MESH AND OPERATING CONDITIONS

The combustion chamber for the simulated engine was generated using ABAQUS software. The geometry was partitioned into distinct surfaces using STAR-CCM+ software, effectively separating the valves, ports, and piston crown from one another (Figure 5).

The computational grid (Figure 6) comprised the cylinder volume, inlet, and exhaust ports. Different grid shapes were employed for each component to optimize solution time and enhance grid quality. The grid for the cylinder primarily consisted of hexahedral-shaped cells, while the grids for the intake and exhaust ports consisted of a mix of hexahedral and tetrahedral cells. Hexahedral shapes provided more accurate solutions with minimal computational time. The determination of the total number of cells in the computational grid took into consideration factors such as cell quality, solution time, and the maximum cylinder pressure. At Bottom Dead Center (BDC), the grid comprised approximately 168,448 cells. A grid independence test was conducted, and it was found that using 168,448 cells for the cylinder volume, inlet, and exhaust ports at BDC consistently produced reproducible results.

Table 7 and Figure 7 present the computational time and maximum cylinder pressure for 4 different cell numbers.

The moving mesh, which includes regions for the piston and intake valves, as well as the initial and boundary conditions, were supplied by ESICE and CD-Adapco's specialized tool designed to facilitate transient analyses of internal combustion engines.

3.1 | Numerical analysis models

The STAR-CD-ESICE codes were employed for solving the discretized Navier-Stokes equations in this study. To characterize combustion,

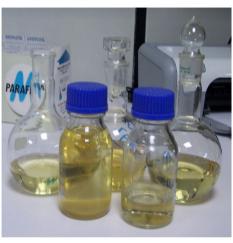




(b)

FIGURE 4 Biodiesel Production
(a) Production setup (b) Methanol separation (c) Purification (d) Products.





(d)

the ECFM-3Z combustion model was utilized. This model, developed by Colin and Benkenida³⁵ encompasses premixed and partially premixed combustion, while also being adaptable for modeling unpremixed combustion. It incorporates three distinct mixing zones: one for pure fuel, another for pure air and possible residual gases, and a mixed zone where the Extended Coherent Flame Model (ECFM) model is applied. The ECFM-3Z model includes auto-ignition, premixed, and diffusion combustion. ECFM-3Z combustion model is based on the flame surface density equation, which takes into consideration the wrinkling of the front surface flame due to turbulent fluctuations and utilizes the conditioning averaging technique. The model can be described as a simplified Conditional Moment Closure type model, where the mixing ratio space is represented by only three points. Reitz-Diwaker model³⁶ was used to characterize droplet break-up, while Huh's model was used to model atomization.³⁷ In this study, the widely recognized Re-Normalization Group (RNG) k-ε model was adopted for turbulence modeling, offering the advantage of accounting for swirl effects. Fuel injection was executed using the Lagrangian multiphase droplets model, while Bai's spray impingement model was applied as the discrete-phase wall interaction model.³⁸ The Zeldovich mechanism was selected to represent NO_x emissions.

4 | RESULTS AND DISCUSSION

4.1 | Experimental results

Figure 8 illustrates the results of the performance experiments conducted on both Diesel fuel and biodiesel within the range of 1600–3000 rpm, with intervals of 200 rpm, and under full engine throttle conditions. The peak torque was attained at 1800 rpm in the test engine for both Diesel fuel and biodiesel. Between 2400 and 3000 rpm, the engine brake power and torque of Diesel fuel outperformed that of biodiesel, exhibiting a maximum discrepancy of 5%. The reduction in torque beyond the 1800 rpm can be explained by the rise in frictional losses and the reduction in volumetric efficiency. It could be said that the engine power of biodiesel and diesel remained comparable between 1600 and 2400 rpm. Nevertheless, post the 2400 rpm, owing to the superior calorific value and lower viscosity of diesel, more effective combustion occurred, consequently resulting in higher engine brake power for Diesel fuel compared to biodiesel.

As seen in Figure 8c, it was observed that when biodiesel was utilized across all assessed speeds, the specific fuel consumption

applicable Creative

TABLE 4 Fuel specifications to be employed as fuel for experimental study.

Proportion	Discol Fuel	Diadiasal
Properties	Diesel Fuel	Biodiesel
Density (kg/m³)	838.2-ISO 12185	883.7-ISO 12185
Kinematic Viscosity (mm ² /s)	2.729-EN ISO 3104	4.482-EN ISO 3104
Total Contamination (mg/kg)	< 6-EN 12662	1.50-EN 12662
Cetane Number	51.5-EN ISO 5165	55.5-EN ISO 5165
Oxidation Stability (h)	4-EN ISO 12205	10.47-EN ISO 12205
Flash Point (°C)	65.5-EN ISO 2719	176-EN ISO 3679
Cold Filter Plug Point (°C)	-11-EN116	-10-EN116
Monoglycerol (m/m) %	-	0.52-EN 14105
Diglycerol (m/m) %	-	0.07-EN 14105
Triglycerol (m/m) %	-	< 0.10-EN 14105
Free glycerol (m/m) %	-	< 0.06-EN 14105
Total glycerol (m/m) %	-	< 0.144-EN 14105
Ester (m/m) %	-	97.8-EN 14103
Linolenic acid methyl ester (m/m) %	-	9.17-EN 14103
Carbon content (m/m %)	< 0.1-ISO 20847	0.130-EN ISO 10370
Water content (mg/kg)	85-EN ISO 12937	440-EN ISO 12937
Ash content (m/m%)	0.0015-EN ISO 6245	0.002-ISO 3987
Sulfur content (mg/kg)	809-ISO 8754	10-ISO 20846
Copper strip corrosion	1a-EN ISO 2160	1a-EN ISO 2160
Acid number (mg KOH/g)	-	0.46-EN 14104
Fatty acid methyl ester (V/V%)	< 0.05-EN 14078	-
Polycyclic aromatic hydrocarbon (m/m%)	5.6	- EN 12916
Lubrication (μm)	309-EN ISO 12156-1	-
Distillation		-
250 °C -V/V	36.1-EN ISO 3405	
350 °C - V/V	94.7-EN ISO 3405	
95% evaporated at (°C)	351.5-EN ISO 3405	

Note: Analyzed at laboratory of TUBITAK MRC.

surpassed that of Diesel fuel. Upon analyzing the fuel properties, it was deduced that heating value (HV) for diesel fuel and biodiesel stood at 42.86 and 38.81 kJ/g respectively. 9.5% decrease heating value of biodiesel contributed to the up to %16.9 increase in SFC and decrease in power and torque. The brake power values of biodiesel was reduced by up to 6.7% between 3000 and 2600 rpm due to HV and higher viscosity and density in comparison to diesel fuel and increased maximum 1.4% between 1600 and 2000 rpm. It was observed that torque loss was 7.1% when pure biodiesel was used as

TABLE 5 Biodiesel specifications for numerical analysis.

Blodieser specifications for flumerical	ariary 515.
Biodiesel-Methyl Oleate (C ₁₉ H ₃₆ O ₂)	
Liquid	
Density ^a (kg/m ³)	883.7
Molecular weight (kg/mol)	296
Boiling temperature (°K)	617
Critical temperature (°K)	764
Formation temperature (°K)	298
Cetane number ^a	55.5
Molecular viscosity ^a (kg/ms)	3.89E-3
Surface tension N/m	0.3786
Specific heat capacity (J/KgK)	1937
Thermal conductivity (W/mK)	0.09985
Saturation pressure (Pa)	2.141E-2
Heat of vaporization (J/kg)	217,000
Lower heat value ^a (kJ/g)	38.81
Gas	
Heat of formation (J/kg)	-2111E+06
Density (kg/m³)	6.237
Molecular weight (kg/mol)	296
Thermal expansion coefficient	0
Temperature of formation (°K)	298
Molecular viscosity (kg/msn)	6.82-6
Specific heat capacity (J/KgK)	2582
Thermal conductivity	0.04065

^aAnalyzed at laboratory of TUBITAK MRC according to TS EN 14214 standards.

fuel instead of diesel at 3000 rpm. Researchers generally agree that due to the HV of biodiesel, engine power decreases. $^{39-45}$

In order to investigate the break torque of the test engine, Hansen et al^{42,46} changed some parameters such viscosity, density, and fuel heating value. They discovered that using 100% biodiesel instead of D2 diesel at an engine speed of 1900 rpm, resulted in a 9.1% reduction in break torque. According to Utlu et al⁴¹ biodiesel fuel has an LHV reduction of about 8.8%.

ECE R 96-05 Stage V emission standards for nonroad are presented in Table 8.

The standard emission levels for nonroad engines (between 8 and 19 kW).

Figure 9 illustrates the findings related to emissions. Upon analyzing the $\rm CO_2$ and $\rm O_2$ emissions, It becomes evident that the emission values from biodiesel were greater. This higher emission can be attributed to the increased oxygen content within biodiesel, leading up to 16.6% rise in $\rm O_2$ and up to %4.4 reduction in $\rm CO_2$ emissions. Furthermore, the higher cetane number and oxygen content of biodiesel led to an enhanced combustion process, subsequently leading up to 32.3% reduction in $\rm CO$ emissions. Conversely, the temperatures of exhaust gases depend on the combustion quality within the cylinders. It could be said as the combustion improves the

GC specifications of biodiesel.

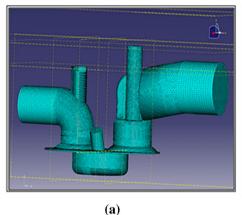
C Number	Mass %	Mass %	Molecular weight (MW)	MW ^a Mass %
Citallibei	141033 70	141033 70	Weight (IVIVV)	141033 70
C12	0.01022	0.000102	214.31	0.0219
C14	0.06135	0.000613	242.36	0.1486
C16.0	4.58078	0.045807	270.43	12.387
C16.1	0.224958	0.002249	268.43	0.6038
C18	1.84049	0.018404	298.48	5.4935
C18.1	60.21472	0.602147	296.46	178.51
C18.2	20.75665	0.207566	294.45	61.118
C18.3	9.64213	0.096421	292.43	28.197
C20.1	1.22699	0.012269	324.00	3.9754
C22.1	0.07157	0.000715	352.57	0.2523
C22	0.910020	0.009089	354.57	3.2227
C20.2	0.03064	0.000306	322.00	0.0986
C20.3	0.14	0.001429	320.00	0.4575
C24	0.13276	0.00132	382.62	0.5079
C24.1	0.153319	0.00153	380.62	0.5830
Average Ma	ss			295.586

^aAnalyzed at laboratory of TUBITAK MRC.

temperature increase, as indicated in Figure 9c. The abundance of oxygen in biodiesel (specifically canola oil methyl ester) facilitated more effective combustion, causing up to 24.4% increase in exhaust temperatures. Notably, NO emissions from biodiesel were elevated between the engine speeds of 1600 to 1800 rpm and 2800 to 3000 rpm up to 8.6%.

According to some authors 40,41,47,48 biodiesel produced less CO₂ than diesel oil because of its lower carbon to hydrogen ratio. Lin and Lin⁴⁹ compared the CO₂ emissions from three different types of biodiesels using ASTM No. 2D diesel. According to Lin and Lin, 49 the three various types of biodiesel had lower CO2 levels than the diesel stated. This difference can be explained by the fact that biodiesel has less carbon than regular diesel fuel and has a lower elemental carbonto-hydrogen ratio. Several studies have found that pure biodiesel reduces CO emissions. 40-43,50-60

Ozsezen et al,40 observed that CO emissions exhibited a reduction range of 86.89% and 72.68% for Waste Palm Oil Methyl Ester (WPOME). Raheman and Phadatare, 43 noted 73%-94% reduction in CO emissions for pure karanja methyl ester (B100) and its blends (B80, B60, B40, and B20) in comparison to diesel oil. Krahl et al,61 identified a reduction of approximately 50% in CO emissions when employing vegetable oil biodiesel as opposed to ultra-low and low-



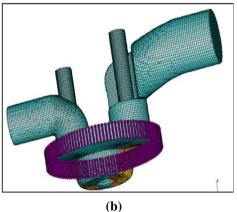
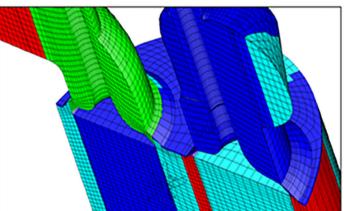


FIGURE 5 Meshing (a) surface mesh of combustion chamber (b) combination of engine parts.



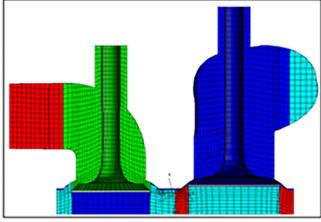


FIGURE 6 Computational grid.

TABLE 7 Maximum cylinder pressure for different grids.

	Low Coarse Mesh	Coarse Mesh	Intermediate Mesh	Fine Mesh	Very Fine Mesh
Cell number	75,000	120,000	168,448	250,000	400,000
In-cylinder maximum pressure (bar)	-	53.08	69.61	69.61	69.61
Solution duration (h)		24	36	63	80

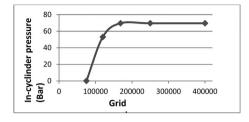


FIGURE 7 Maximum cylinder pressure for different grids.

TABLE 8 The standard emission levels for nonroad engines.

	Net Power		g/kWh	1		
Category	kW	Date	со	НС	NOx	PM
NRE-v/c-1	8 < P	2019	8.00	7.50 ^{a,0}		0.40 ^b
NRE-v/c-2	8 ≤ P < 19	2019	6.60	7.50 ^{a,0}		0.40

 $^{^{}a}HC + NOx.$

 $^{^{}c}A = 1.10$ for gas engines.

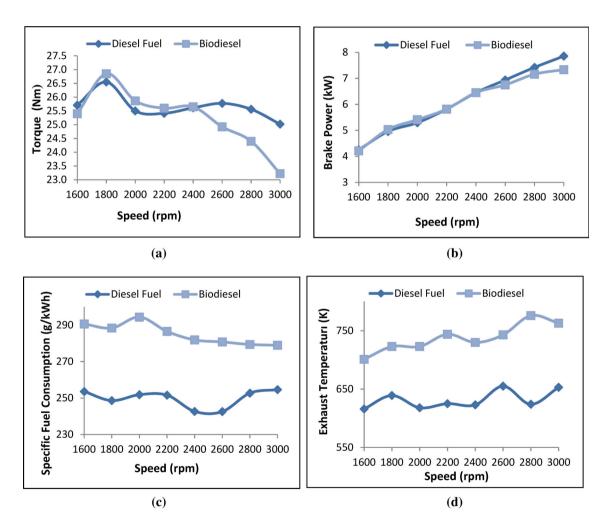


FIGURE 8 Experimental performance results (a) Torque (b) Brake power (c) Specific fuel combustion (d) Exhaust temperature.

sulfur diesel. Utlu and Koçak⁴¹ obtained a CO reduction of 17.3%, while Puhan et al⁶² achieved a decrease of about 30%. Nonetheless, a number of studies found no reasonable difference in CO emissions between diesel and biodiesel.^{63,64}

Some researchers have noticed an important increase in CO emissions from pure biodiesel. ^{57,65-67} The CO emissions for HOME, SOME, and JOME in a 1-cylinder, 4-stroke, WC, DI, and CI diesel engine at 1500 rpm were compared by Banapurmath et al. ⁶⁶ For

^b0.60 for hand-startable, air-cooled direct injection engines.

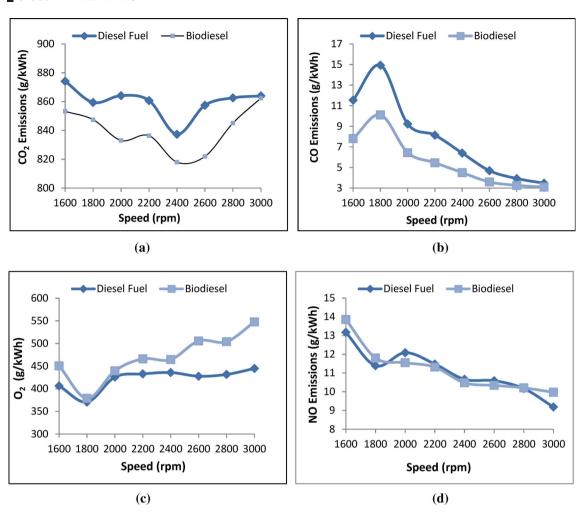


FIGURE 9 Experimental emission results (a) CO₂ emissions (b) CO emissions (c) O₂ emissions (d) NO emissions.

TABLE 9 Numerical analysis parameters between 3000 and 2400 rpm for biodiesel.

Numerical Analysis Parameters	3000	2800	2600	2400
Injection duration (°CAD)	14	15	16	17
Injection advance (°CAD)	14	13	12	11
Injection flow rate (kg/s)	0.0292	0.027	0.024	0.021
Droplet number	45,000	40,000	39,000	35,000
Max pressure (bar) @deg.CA	69.15@366.4	69.96@367.5	66.11@368.4	63.32@369.6

HOME, JOME, and SOME, the CO values were 0.145%, 0.155%, and 0.12%, respectively, but the diesel value at 80% running load was 0.11255%. Pure biodiesel extracted from jatropha oil had a declining CO emission, ⁴⁷ but pure biodiesel extracted from polanga and karanja oil showed a noticeable variation. In particular, Fontaras et al⁶⁵ reported using B100 and B50 increased CO emissions above the new European driving cycle by approximately 54% and 95%, respectively.

It was observed that most of studies indicate a rise in NO_x emissions when pure biodiesel is employed 42,47,56,57,64,68 due to higher gas temperature in combustion chamber with 12% oxygen content in product gas. 67 Ozsezen et al, 40 conducted research on a 6-cylinder

direct injection, naturally aspirated, water-cooled diesel engine using WPOME. They found that the NO_x emissions from WPOME increased by 6.48% and 22.13%, respectively. Durbin and Norbeck⁶⁹ investigated pure biodiesel, conventional diesel, and blends containing 20% biodiesel in four distinct engines. They found no reasonable variation in NO_x emissions and concluded that the disparity was not significant. Puhan et al,⁶² demonstrated that using methyl oleate ethyl ester led to a 12% reduction in NO_x emissions across the entire load range when compared to diesel fuel. In the other study, Dorado et al,⁷⁰ observed a 20% decrease in NO_x emissions when using waste olive oil biodiesel across 8 different mode cycles.



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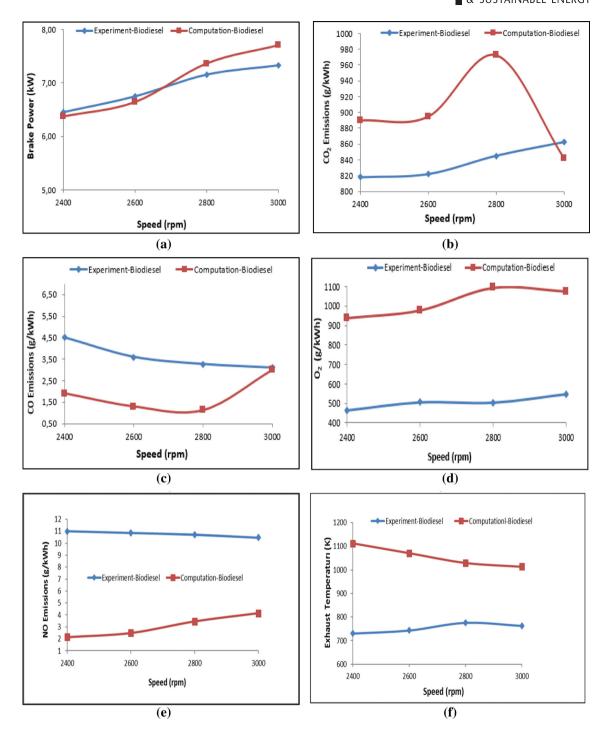


FIGURE 10 Experimental and numerical results (a) Brake Power (b) CO_2 emissions (c) CO emissions (d) CO emissions (e) CO emissions (f) Exhaust temperature.

4.2 | Numerical results

Since the injection advance and injection duration were 14°CAD and 17°CAD respectively in the engine tests carried out at 3000 rpm at Anadolu Motor, the simulation investigation was initiated using diesel fuel (hepta methyl nonane) under these actual engine conditions. 72 bar was the highest experimental in-cylinder pressure for diesel fuel. By adjusting the spray advance, spray time,

spray volume, and number of droplets sprayed from each injector, it was attempted to approach the power value attained in the experiments for each cycle, since the emission values were compared per unit energy (g/kWh).

Numerical analysis parameters between 3000 and 2400 rpm are shown in Table 9.

Injection advance and injection duration were selected as 14°CAD for biodiesel at 3000 rpm. As the revolutions decrease by

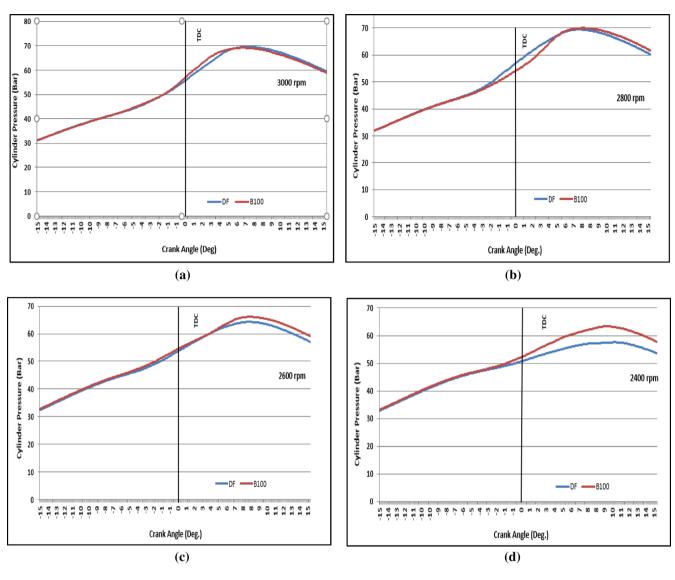


FIGURE 11 Variation of cylinder pressure at different crank angles (a) 3000 rpm (b) 2800 rpm (c) 2600 rpm (d) 2400 rpm.

200 rpm, injection duration was increased by 1°CAD and the advance value was reduced by 1°CAD in the numerical study. It was observed that combustion did not occur when the quantity of droplets was excessively high. Because of this, the optimum number of droplets was determined in each cycle. Due to the higher viscosity and density of biodiesel, the number of droplets was higher at combustion of diesel fuel. The amount of fuel injected from the injectors was obtained from the test results. The exhaust gas calculations were computed in the numerical analysis when the exhaust valve was opened. The experimental study and the ECFM-3Z performance findings were compared. Figure 10 shows the power and emission findings of experimental and numerical studies at full load speed, between 3000 and 2400 rpm.

In the comparison between the ECFM-3Z combustion model and the experimental study for biodiesel at different rpm levels, the brake power value showed differences. 2400 rpm, the numerical analysis showed a 1.2% higher power value than the experimental study, while at 2600 rpm, it was 1.6% less. However, at 2800 rpm, the numerical analysis indicated a 2.81% higher brake power value compared to the experimental study. Finally, at 3000 rpm, the numerical analysis displayed a 5% higher brake power value than the experimental study. The brake power values of the experimental and numerical investigations for biodiesel were extremely close to each other, as Figure 10a illustrates.

In terms of emissions and exhaust temperatures significant differences were observed. At 2400 rpm, CO2 emissions were within the error band (%4.19), with NO and CO emissions being 84.4% and 57.8% lower, respectively. There were notable increases of 52.3% and 101.5% in exhaust temperatures and O2 emissions, respectively. At 2600 rpm, CO and NO emissions were substantially lower by 64.2% and 80.8%, while CO₂ emissions increased by 8.8% and O₂ levels increased by 93%. Additionally, the numerical analysis showed 44.1% higher exhaust temperatures. Similarly, at 2800 rpm, CO and NO emissions were significantly lower by 65.6% and 71% respectively, while CO2 and O2 emissions increased by 15% and 117%



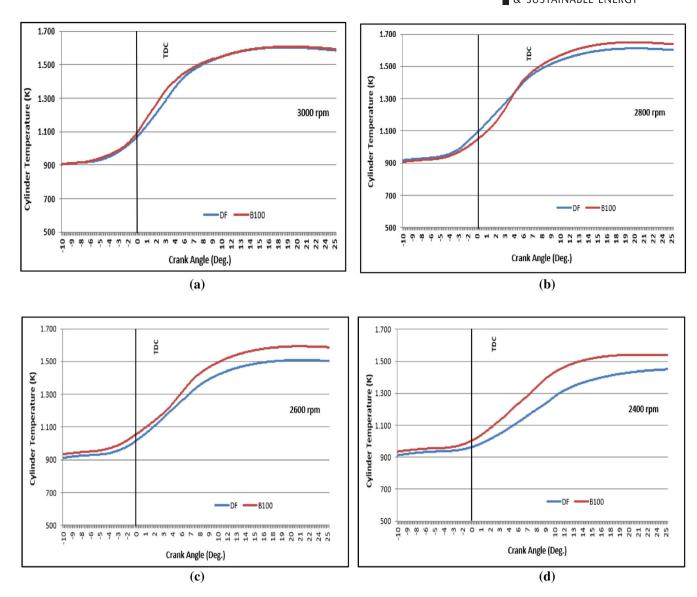


FIGURE 12 Variation of cylinder temperature at different crank angles (a) 3000 rpm (b) 2800 rpm (c) 2600 rpm (d) 2400 rpm.

respectively. Moreover, there was a 32.7% increase in exhaust temperatures. Finally, at 3000 rpm, O_2 emissions were 96.4% higher, while CO_2 and CO emissions were within the error band (%4.20 and %4.12 respectively). Notably, there was 63.4% less NO released compared to the experimental study, and the numerical analysis showed a 32.9% increase in exhaust temperatures.

4.2.1 | Combustion characteristics

The combustion characteristics of biodiesel was analyzed and compared with the baseline diesel fuel. Specifically, the analysis focused on in-cylinder pressures and temperatures under 2400–3000 rpm at full load conditions to evaluate combustion parameters.

Figure 11 shows the variation in cylinder pressure versus crank angle under 2400–3000 rpm at full load conditions. It can be observed that at 3000 rpm, the highest pressure recorded in diesel

fuel was 69.62 bar at 7.0 CAD, while in biodiesel, it reached 69.16 bar at 6.4 CAD. The peak pressures for both biodiesel and diesel fuels were comparable and occurred at approximately the same location. Moving to 2800 rpm, the maximum pressure in diesel fuel was 69.41 bar at 7.2 CAD, and in biodiesel, it was 69.96 bar at 7.7 CAD. The maximum pressures for biodiesel and diesel fuels were identical and observed at the same position. At 2600 rpm, the maximum pressure in diesel fuel was 64.26 bar at 728.3 CAD, while in biodiesel, it was 66.12 bar at 728.1 CAD. The maximum pressures for both biodiesel and diesel fuels were similar and occurred in the same location. Finally, at 2400 rpm, in the simulation study for diesel fuel, the maximum pressure was 57.58 bar at 10.4 CAD, and for biodiesel, the maximum pressure was 63.32 bar at 9.6 CAD. Biodiesel reached its maximum pressure earlier and exhibited a higher value.

As seen in the Figure 12 cylinder temperatures of biodiesel are slightly higher than diesel. However, the peak points are almost the same.

5 | CONCLUSIONS

This research highlights the importance of being able to characterize and compute biodiesel fuel properties, thereby providing a biodiesel fuel definition that can be used in any numerical analysis.

The main conclusions are summarized below:

- C₁₉H₃₆O₂ was predicted as a single component surrogate biodiesel. It was determined according to % fatty acid concentrations and average mass calculation. The results of the model show the applicability of methyl oleate for biodiesel surrogate fuel.
- ECFM-3Z brake power results are in close agreement with experimental study. Considering the uncertainty values in the 3000–2400 rpm range, there is a maximum difference of 5% in the performance of biodiesel. This value is within acceptable limits. This difference can also be caused by keeping the injection advance constant in experimental studies.
- CO₂ emissions were compatible with experimental study. There was max 10% difference.
- CO emissions were 57%-65% lower than experimental study.
- O₂ emissions were 93%–117% higher than experimental study.
- NO emissions were 63%-84% lower than experimental study.
- Exhaust temperatures were 33%-49% higher than experimental study.

The research on biodiesel combustion characteristics provides valuable insights that can directly benefit companies in the automotive and transportation sectors. These results provide insight into the possible advantages and shortcomings of the ECFM-3Z method for evaluating the emissions and performance of diesel engines powered by biodiesel. The findings can help enhance engine designs, improve efficiency, and promote cleaner technologies in industries. Engine manufacturers and researchers can use the knowledge gained to optimize engine designs, fuel injection strategies, and combustion processes for biodiesel. This can lead to better fuel efficiency, reduced emissions, and more sustainable engine operation. Furthermore, the study validates the ECFM-3Z model using experimental data in terms of performance. It provides valuable tool for the industry to conduct further simulations and optimize engine performance with biodiesel. As the demand for sustainable and environmentally friendly fuel alternatives grows, the study's findings can contribute to the development and widespread adoption of biodiesel as a cleaner and renewable fuel source in the transportation sector. However, it is recommended to carry out detailed studies by using various surrogate fuels, spray break up, atomization and droplet models for emissions. Future studies could focus on investigating the effect of other biodiesel feedstocks on the engine's performance and emissions. It would also be interesting to investigate the impact of different injection strategies, such as multiple injections or pilot injections, on the combustion and emissions of biodiesel.

AUTHOR CONTRIBUTIONS

Şeyma Karahan Özbilen: Writing – original draft; investigation; methodology; validation; software; conceptualization; writing – review and

editing; formal analysis; visualization. **Emrullah Hakan Kaleli**: Supervision; conceptualization. **Emir Aydar**: Software; investigation; methodology; visualization.

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CONFLICT OF INTEREST STATEMENT

No potential conflict of interest was reported by the author(s).

DATA AVAILABILITY STATEMENT

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

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