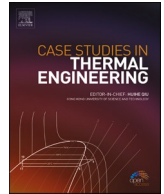




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Enhancing CI engine performance and emission control using a hybrid RSM–Rao algorithm for ZnO-doped castor–neem biodiesel blends

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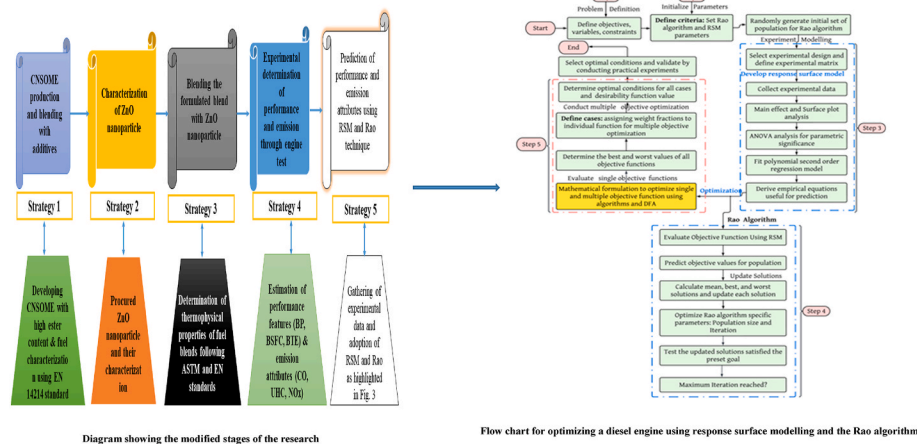
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GRAPHICAL ABSTRACT



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ABSTRACT

Traditional optimization methods, like Response Surface Methodology (RSM) alone, have failed to capture the complexities of engine operation, leading to the adoption of a more efficient algorithmic approach that requires no algorithm-specific parameters. Additionally, biodiesel produced from a single oil has not only failed to enhance performance effectively but has not maintained a benign environment, resulting in high emission tail, most importantly NO_x. For the first time, the study adopts RSM and the Rao-3 Algorithm, a population-based metaheuristic, to optimize and model the performance and emissions attributes of a CI engine running on a ZnO-doped composite biodiesel (CB) blend, adopting neem-castor biodiesel as CB. The former algorithm possesses the aforementioned features. Rao's algorithm does not mimic the behaviour of swarms, animals, birds, or any physical or chemical phenomenon, but it provides effective solutions to complicated problems. For the first time, the study adopts the hybridization of the RSM and Rao 3 algorithm to model and predict the IC engine operated on composite biodiesel/castor-neem seed oil methyl ester (CNSOME)/diesel/ZnO blends. This involves the impact of input engine variable ranges such as fuel blends (10–40 v/v%), ZnO dosage (20–100 ppm), engine speed (800–2000 rpm), and engine load (10–40 %) on performance indices (PI) such as brake power (BP), and brake thermal efficiency (BTE) and emission attributes (EAs) namely carbon monoxide (CO), unburnt hydrocarbon (UHC), oxide of nitrogen (NO_x) as responses. RSM was used to plan the design of the experiment and detect the optimal engine conditions for enhancing PI and reducing EAs while 3 algorithms were used to solve a multi-objective function. The results show that the RSM model determined optimal condition resulted experimentally the BP of 7.3 kW, and BTE of 25.96 % and CO of 64.5 ppm, UHC of 2.64 ppm, and NO_x of 705.4 ppm were attained at a fuel blend of 21.34 % vol., ZnO additive of 61.35 ppm, engine load of 21.5 %, and engine speed of 1380 rpm correspond to case 5 determined highest desirability function value of 0.9553. Rao-3 algorithm provides the optimal parametric condition (21.34 vol% of blend fuel, 63.43 ppm of nanoparticle, 1435.18 rpm of engine speed, and 24.35 % for engine load) with a desirability function approach (DFA) value equal to 0.9556, and were subjected to conduct practical experiments. Experiments corresponding to case 5 (21.34 vol% of blend fuel, 64 ppm of nanoparticle, 1435 rpm of engine speed, and 24 % for engine load) resulted in BP, BTE, CO, UHC, and NO_x equal to 8.2 kW, 29.4 %, 66.2 ppm, 2.82 ppm, 701.4 ppm, respectively. The performance of the Rao algorithm seems to be superior to the RSM because the deviation in Rao algorithm predictions with experimental values resulted in an absolute percent error equal to 4.63 % for BP, 3.98 % for BTE, 2.46 % for CO, 5.32 % for UHC, and 0.85 % for NO_x emissions, respectively. The hybrid models using RSM-Rao-3 algorithms can be a robust model to enhance performance and reduce the emission profile of an IC engine powered by a novel green diesel derived from a myriad of generations without being trapped at local minima solutions. It obtains the best solution through iteration. This study presents an innovative framework for biodiesel

engine optimization, contributing to the advancement of sustainable and efficient green diesel technologies.

1. Introduction

Despite the driving forces to reduce carbon emissions, internal combustion engines (ICs) remain important for industry and transportation. Biodiesel is a promising alternative to fossil fuels as it is renewable, biodegradable, and emits fewer greenhouse gases. Neem and castor oil from non-specific sources provide sustainable options for biodiesel production and reduce the need for food harvesting competition. The reduction in performance of biodiesel compared to diesel requires the use of performance enhancers. Including nanoparticles in the biodiesel compound helps to reduce emissions. The oxygen-containing properties of nanoparticles are effective in improving emission reduction and a variety of nanoparticles can be used for this purpose, including commonly used nanoparticles such as cerium oxide, titanium aluminum oxide, copper oxide, and carbonanth. Among these, ZnOs are preferred for their ability to improve the occurrence of micro-explosions, increase oxygen levels, increase ignition speeds, and improve fuel combustion.

Conventional techniques such as One-Variable-At-A-Time (OVAT), Taguchi methods, and Artificial Neural Networks (ANN) have led to unreliable predictions. For instance, OVAT ignores the interaction effects between variables and is deficient in recognizing complex interactions and nonlinear relationships between variables. The Taguchi method focuses predominantly on robustness but may not adequately explore the entire design space and often fails to recognize complex interactions and nonlinear relationships between variables. ANN requires large datasets for accurate training and lacks transparency and interpretability in prediction mechanisms due to its “black box” approach. Additionally, the current techniques and existing approaches lack the capacity to capture the multidimensional, nonlinear, and interactive nature of the problem space, which is crucial for optimizing conditions in complex systems. Due to unreliable predictions and the failure to optimize conditions in complex systems, researchers, scientists, and stakeholders have shown interest in obtaining hybrid models that systematically synergize multiple input variables to establish reliable predictions and effective modeling. Among the computational techniques, RSM and metaheuristic optimization algorithms like the Rao algorithm, offer powerful tools for modelling and optimizing multi-input vs. multi-response datasets. Hybridizing RSM with metaheuristic algorithms, such as enhanced global optimization, improves prediction accuracy, efficient handling of multi-response optimization, reduces experimental costs, provides flexibility, scalability, improved robustness, and applicability across complex systems [1–3].

1.1. Theory, utility, and adaptability of RSM and Rao approaches

RSM employs mathematical modeling to estimate the connection between input and output variables, aiming to enhance responses. Rao algorithms prioritize mathematical principles for optimization, avoiding intricate processes. Unlike nature-inspired metaheuristics, Rao algorithms employ fundamental arithmetic operations to progressively improve solutions.

The Rao-RSM model is a hybrid approach that integrates. On the other hand, Rao algorithms and RSM are used to tackle optimization problems in intricate, high-dimensional, and nonlinear systems. This model offers a reliable and flexible solution by utilizing the global optimization capabilities of Rao algorithms and the local modeling of RSM. The Rao-RSM model offers several advantages, such as improved optimization efficiency, lower experimental expenses, the ability to handle multiple objectives, and its applicability in complex and nonlinear systems, as well as data-driven decision making.

1.2. Motivation, knowledge gaps, and aim of the study

Extensive research has been conducted using parametric studies to analyze the performance and emission characteristics of IC

Table 1
Engine optimization for composite biodiesel blends.

Types of feedstock	NA	Performance	Emission	RSM	ONVAT	Rao	Remarks
CPMLAI	✓	✓	✓	✓	NS	×	[4]
PPCO	×	✓	✓	✓	×	×	[5]
PPJO	×	✓	✓	✓	×	×	[6]
CHCO	×	✓	✓	×	✓	×	[7]
LRSO	×	✓	✓	×	✓	×	[8]
SUSO	×	✓	✓	✓	×	×	[9]
PCIO	×	✓	✓	×	✓	×	[10]
CHSO	×	✓	✓	✓	×	×	[11]
PJO	×	✓	✓	×	×	×	[12]

× = Absent; ✓ = Present; NS= Not study ✓ = ✓

engines fueled by blends of composite biodiesel. RSM has been employed to enhance these qualities across different types of fuel. Table 1 summarizes engine features operated on hybrid fuels such as Ceiba Pentandra, Mahua Longifolia, and Azadirachta Indica (CPMLAI) [4], plastic pyrolysis oil and coconut oil (PPCO) [5], pumpkin and Prosopis juliflora oil (PPJO) [6], cooking oil and Hibiscus Cannabinus (CHCO) [7], linseed and rubber seed oil (LRSO) [8], sunflower and soybean oil (SUSO) [9], palm and *Calophyllum inophyllum* oil (PCIO) [10], canola-hazelnut soapstock oil (CHSO) [11], and palm and jatropha oil (PJO) [12].

Table 2 provides an overview of studies on biodiesel from castor and neem seed oil (CNSO), including esterification and transesterification [13], tribological analysis [14], pretreatment methods [15], CNSO as a cutting fluid [16], OVAT-based engine testing [17], empirical fuel property estimation [18], OVAT-based partial engine testing of CNSO methyl ester [19], and CNSO-based lubricity assessment in machining steel [20].

Tables 3 and 4 further summarize hybrid optimization techniques for IC engines and Rao-based optimization in engineering applications, respectively. As seen in Table 3, Fareed et al. [21] experimentally investigated waste–palm oil biodiesel in IC engines, while Viswanathan et al. [6] assessed pumpkin-Prosopis-Rudraksha biodiesel. However, Rao-based prediction models remain unexplored. Table 4 details Rao algorithm applications, including composite engineering [22], water network pipe sizing [23], mining operations [24], renewable energy integration [25], traffic network modeling [26], sustainable cooling for milling processes [27], heat exchangers [28], dome structures [29], thermodynamic cycles [30], bioenergy systems [31], and machining processes [32]. A comprehensive literature review indicates that the optimization of IC engines using RSM has been extensively researched, primarily employing OVAT-based testing. Nevertheless, OVAT testing may not accurately identify relationships between multiple responses and input variables. The Rao algorithm, frequently employed in engineering fields, is often overlooked for its potential in optimizing engine characteristics and minimizing emissions in internal combustion engines. The current limitations of RSM-based optimization involve its dependence on linear or quadratic models, challenges in dealing with multimodal optimization problems, the possibility of model overfitting or under fitting, and vulnerability to noise in experimental data. OVAT testing does not include multi-response analysis and lacks research on nanoparticle doping to enhance fuel performance. Filling these gaps is essential for improving IC engine efficiency and implementing effective emission reduction strategies.

This research combines the Rao algorithm with RSM to enhance the performance of an IC engine, incorporating a blend of diesel and ZnO nanoparticles. The aims of the study include: 1. Achieving the desired outcome by utilizing CCRD to investigate the effects of different fuel blends, dosage levels, engine speeds, and loads on both performance and emissions. 2. Conducting trials and identifying ideal settings with RSM. 3. Utilizing main effect plots, surface plots, and factor analysis to analyze data. 4. Improving Rao-3 algorithm settings for speed and pollution reduction. 5. Describing the most and least desirable outcomes for goals. 6. Optimizing for multiple objectives to achieve both efficiency and environmental benefits. This research integrates machine learning and experimental methods to propel the development of eco-friendly IC engine technologies.

1.3. Fundamental theory of RSM and Rao algorithms

RSM is a mathematical and statistical method employed to model and analyze problems where system responses are affected by multiple input parameters [33]. In the realm of experiments involving IC engines, RSM provides a cost-efficient method to obtain precise outcomes with reduced experimentation, resulting in time and resource savings. This approach utilizes least-squares techniques to enhance responses by establishing connections between input parameters and output responses. For each input parameter of the engine in RSM, it is assumed to be measurable and represented using Eq. (1):

$$Y = f(\varnothing_1, \varnothing_2, \varnothing_3, \dots, \varnothing_n) \quad (1)$$

where Y is the response and $\varnothing_1, \varnothing_2, \varnothing_3, \dots, \varnothing_n$ are engine input variables

The Rao algorithm series was first introduced by Rao in 2020. These algorithms do not require any specific parameters for the optimization process. As a population-based method, Rao algorithms make use of the most promising and least promising solutions

Table 2

An overview of study on biodiesel derived from CNSO.

Area of study	NPs	MTs	Performance	Emission	Production optimizations	Ref.
EST and TR	×	RSM was adopted for EST and TR	×	×	✓	[13]
Tribology study	×	×	×	×	×	[14]
Esterification modelling	×	RSM-ANFIS	×	×	×	[15]
Hybrid for cutting fluid as wear and surface roughness determination	×	×	×	×	×	[16]
ONVAT based engine testing	×	×	✓	✓	×	[17]
PE	×	Linear regression for PE	×	×	✓	[18]
ONVAT adopted for partial engine testing	×	No model tool adopted expected ONVAT	✓	✓	×	[19]
Lubricity assessment & machining of steel	×	×	×	×	×	[20]

MTs: Model tools; EST: esterification; TR: transesterification, × : Not investigated; ✓: Investigated.

Table 3

A concise review of hybrid optimization techniques for IC engines.

Biodiesels from hybrid oil	Adopted HOTs	IEV vs. Responses	Remarks	Gaps in knowledge	Ref.
Neem-Castor-ZnO Biodiesel	RSM-Rao-3 Algorithm	Fuel blend, ZnO dosage, engine load, speed → BP, BSFC, BTE, CO, NOx, UHC	Hybrid RSM-Rao approach provides robust optimization	First study using Rao-3 for biodiesel-diesel blends	This Study
PO + WCO	Nils: but Experimental Assessment	Blend ratio, engine load → Combustion, performance, emissions	Hybrid biodiesel blends show improved properties; however, specific fuel consumption increased.	Limited exploration of optimization algorithms for performance enhancement.	[21]
PSO + PJSO + RSO	Hybrid Optimization (Meta-heuristic algorithms, ANN)	Engine load, speed, blend ratio → Brake thermal efficiency, specific fuel consumption, emissions	Hybrid approach achieved significant improvements in performance and emission reductions.	Further research needed on real-time optimization and scalability.	[6]

HOTs: hybrid optimization techniques; IEV: Input engine variables; PO: palm oil; WCO: Waste cooking oil; PSO: pumpkin seed oil; PJSO: Prosopis juliflora seed oil; RSO: Rudraksha seed oil, BP =Brake power.

Table 4

Compares Rao with other prediction tools (PTs) for engineering applications.

Engineering application	Analysis and Optimization tool		Remarks	Refs.
	RaO	PT		
Composite engineering	Yes	RSM	Optimal conditions for enhancing reinforced composite identified using Rao-RSM.	[22]
Water delivery network pipe-sizing project	Yes	Nil	The modified Rao-2 algorithm has prospective for finding the optimal solution.	[23]
Mining operation	Yes	Nil	Rao algorithm used to find ore and minerals in region.	[24]
SSTR	Yes	Nil	The robustness and efficiency of Rao-1 algorithm > Rao-2 algorithm in modelling SSTR	[25]
Traffic Network	Yes	PSO	Rao outperformed PSO	[26]
SCFMP	Yes	RSM, oval rate are responses. GA, JAYA, and Rao	Rao outperformed GA and JAYA	[27]
Heat exchanger	Yes	Variant (SAMP Rao algorithms)	Rao and SAMP Rao algorithm demonstrated superior optimization compared to other algorithms.	[28]
Design of dome structures (DSs)	Yes	Nil	The sturdiness and proficiency of Rao-1 algorithm > Rao-2 algorithm in modelling DSs	[29]
Thermodynamic cycles	Yes	Nil	Rao demonstrated the effectiveness of results obtained through proper analysis.	[30]
Bio-energy systems	Yes	Nil	Rao exhibited higher superiority compared to other advanced optimization algorithm	[31]
Machining processes	Yes	ANFIS and Jaya algorithm	Superiority of RaO was proven over other techniques	[32]

within a population. The iterative process seeks to converge towards the global solutions. In every step, potential solutions are randomly evaluated against each other according to the objective function of the problem. The i^{th} population $[X_i]$ consists of various potential solutions, where $X_{t,i,j}$ denotes the j^{th} design variable of the potential solution i^{th} for the t^{th} iteration. The population is represented by 'n', the number of design variables by 'd', and 'r' as a vector of random numbers. Further information, such as the basic flow chart, and specific pseudo-code details of the Rao algorithm, can be found in other sources [28,29]. The algorithm is based on the following steps

2. Materials and methods

To produce castor-neem seed oil methyl ester (CNSOME)/biodiesel from CNSO (a mixture of neem oil and castor oil from Oyo State and Agri Energy Limited in Kano, Nigeria, respectively), methanol will be used as the solvent, and calcined egg shell and cow bones will serve as the heterogeneous catalysts (HCs). The analysis of FTIR confirmed the presence of functional groups in the catalysts. The spectra showed peaks at $1420.11572\text{ cm}^{-1}$ for the carbonate ion, $1099.56466\text{ cm}^{-1}$ for the sulfate ion, and 670.92081 cm^{-1} for aryl thioethers, suggesting sulfate ion and aryl thioethers ($\phi-S$) ($C-S$ stretch), respectively (See Fig. 1). The findings suggest that the catalyst support material was successful.

This section provides an overview of the study's materials and methods, which involved obtaining ZnO nanoparticles as fuel additives, producing CNSOME through transesterification, preparing blended fuels, and conducting engine testing. Fig. 2 depicts the study's phases.

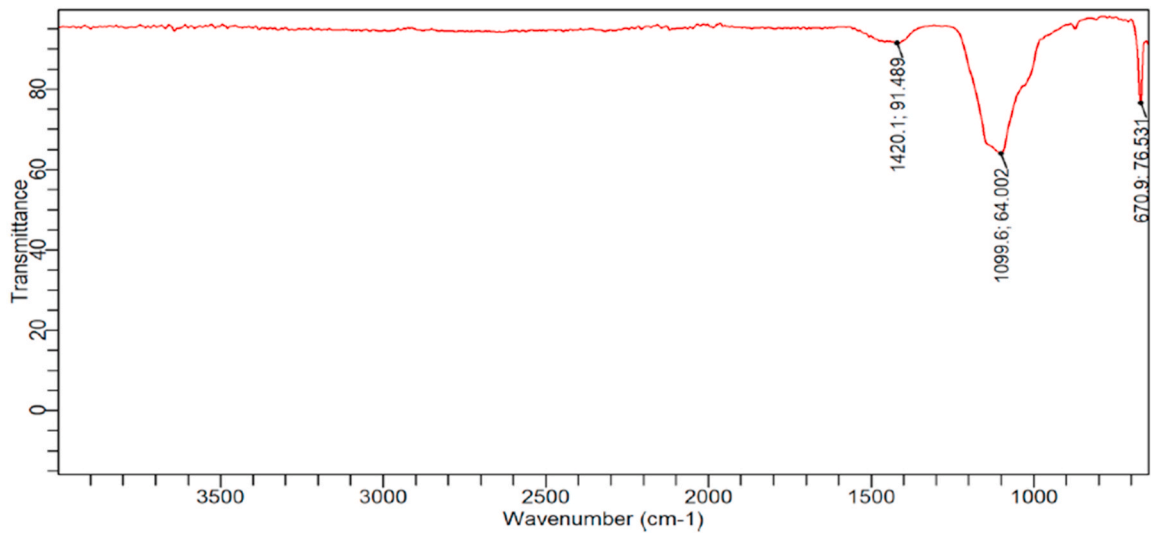


Fig. 1. FT-IR analysis of heterogeneous catalyst synthesized from eggshells and animal bones.

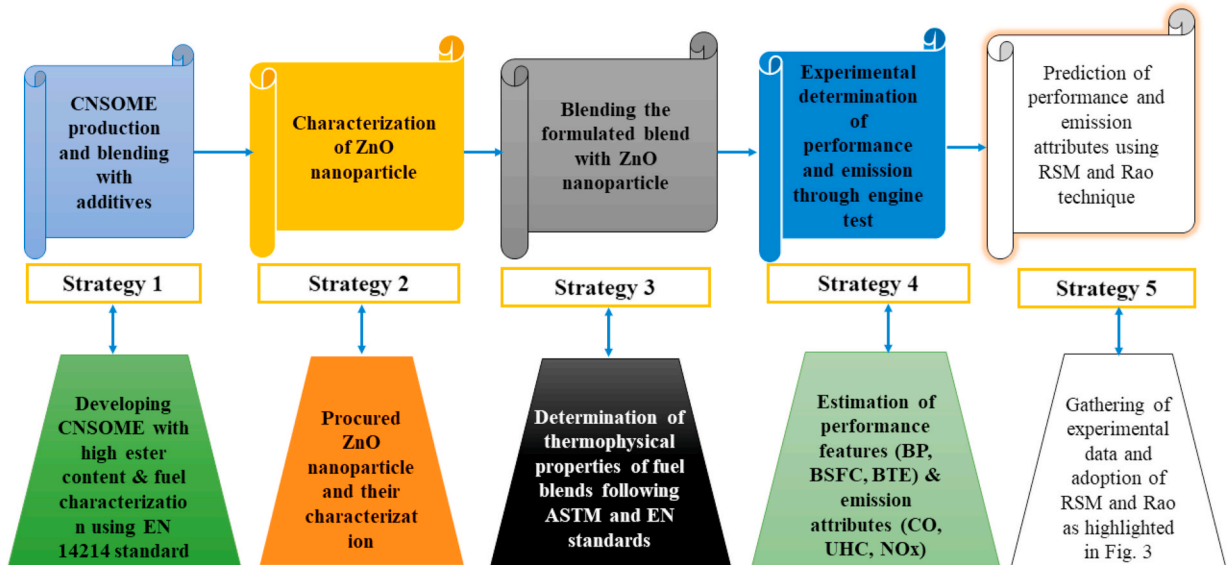


Fig. 2. Diagram showing the modified stages of the research.

2.1. Preparation of CNSOME

Fig. 3 (i-ii) shows the schematic and experimental set-up/pictorial view for producing CNSOME. The transesterification variables (TVs) and methanolysis process for CNSO in this study were chosen based on established transesterification conditions commonly used for inedible oils (Effiom et al., 2024; Samuel et al., 2024). For the esterified CNSO, important variables included the use of a heterogeneous catalyst (HC) in the range of 12–20 wt%, a reaction time (RT) of 1.0–3.0 h, a methanol-to-oil molar ratio of 4:1 to 10:1, and a reaction temperature (RET) maintained between 50 °C and 70 °C. The specific parameters and operating conditions for biodiesel production can be found in Table A1 in Appendix A. Methanol/esterified CNSO of 8.0 is heated to 60 °C for 2 h and mixed using a mechanical stirrer. The mixture (HC-methanol) is vigorously stirred for 2 h and then transferred to a glass container to separate the components from the glycerine. The glycerine is extracted, and the remaining components are rinsed with water to ensure the complete removal of glycerine. The washing process is repeated until there is no glycerin remaining. Finally, the purified biodiesel is heated to 100 °C to eliminate any traces of water, resulting in a high-quality biodiesel product suitable for nano blend preparation. The method is explained in detail in another publication [15].

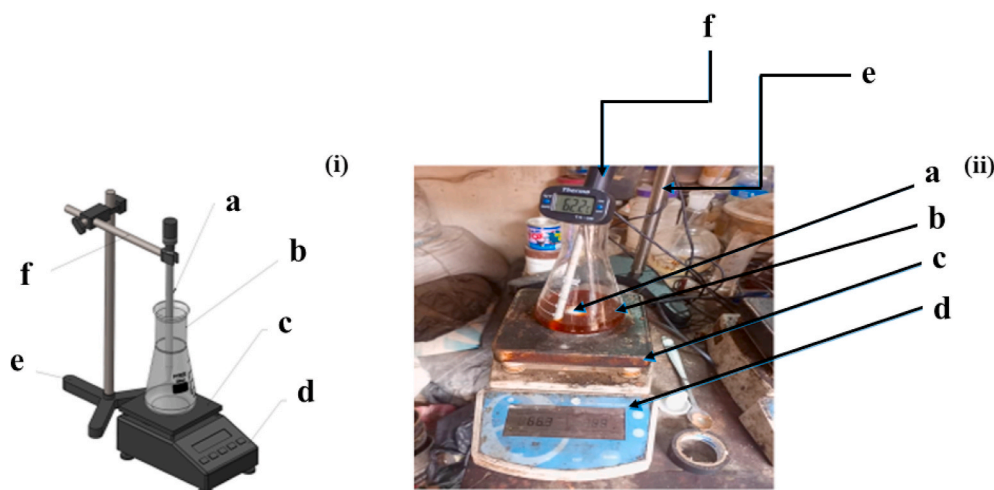


Fig. 3. Biodiesel production process: (i) Schematic set-up and (ii) pictorial view of biodiesel processing equipment: (a) magnetic stirrer, (b) conical flask, (c) hot plate, (d) measuring device, (e) tripod stand, and (f) stirrer holder.

2.2. Preparation and determination of thermophysical properties of ZnO NPs and CNSO biodiesel blend with varying ratios

The nanoparticles (30 nm, 99.9 % purity) were obtained from a laboratory in Nigeria. The nanoparticles were measured using a highly accurate scale (± 0.001 g) and blended using a magnetic stirrer and ultrasonic process, as shown in Fig. 4. Fundamental characteristics of a substance, including density, viscosity, flash point, and calorific values, were determined. Fuel blends (B0ZnO600, B10ZnO400, etc.) were prepared following the standards set by ASTM to assess their thermophysical properties. Table 5a summarizes the basic properties of CNSOME. The flow chart for determining basic properties of the fuel blends is illustrated in Fig. 5. Table 5b presents the flame distribution of certain compounds, while Fig. A1 in appendix 1a illustrates the chromatograph and profile of these compounds. The biodiesel composition is rich in unsaturated fats, especially methyl oleate (40.25 %) and methyl linoleate (29.41 %), which are commonly found in oils such as soybean or rubber seed. Methyl esters such as methyl palmitate (16.33 %) and methyl stearate (8.72 %) are found in smaller quantities, improving ignition quality but slightly affecting cold flow characteristic.

2.3. Methodology for assessing diesel engine performance and exhaust emission

Diesel engine performance attributes such as brake power (BP) and brake thermal efficiency (BTE) as well as exhaust emissions features (EEFs) including carbon monoxide (CO), unburnt hydrocarbons (UHC), and oxides of nitrogen (NO_x) were evaluated on a direct injection (DI) single-cylinder, water-cooled, four-stroke, naturally aspirated test diesel engine model (Zhejiang Sifang). The

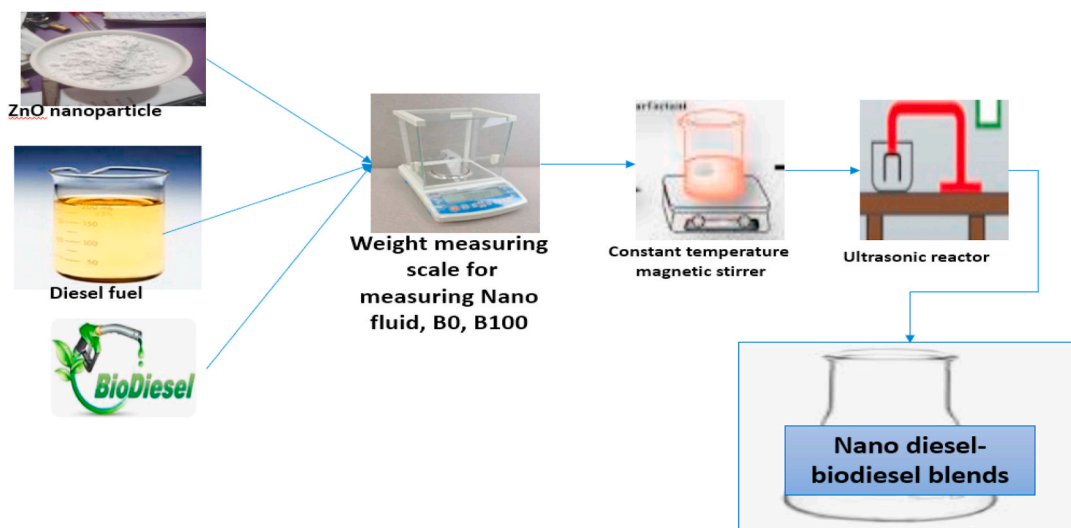


Fig. 4. Schematic for the preparation of nano-fuels.

Table 5a
Fuel properties of CNSOME.

Density @ 40 °C (kg/m ³)	Kinematic viscosity @ 40 °C (mm ² /s)	Flash point (°C)	Acid value (mgKOH/g)	Cloud point (°C)	Pour point (°C)	Sulphur content	Oxidation stability (hr)
808.2	4.128	121	0.38	6.9	3.4	0.0416	75 min

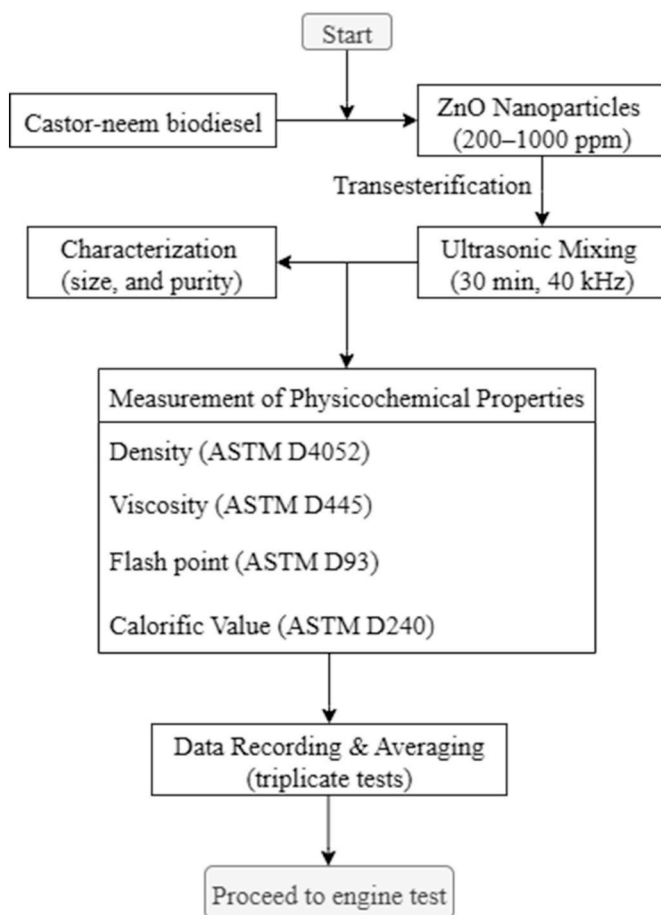


Fig. 5. Flowchart for evaluating ZnO-doped castor-neem biodiesel blends.

Testo 350 XL gas analyzer was employed to measure CO, UHC, and NO_x.

Fig. 6(a and b) shows the pictorial and schematic set-up of a DI diesel engine connected to a hydraulic dynamometer. Varying engine load (10–40 %), engine speed (800–1700 rpm) were generated with varying fuels (0–40 vol% doped with nanoparticle dosage (20–100 ppm) as portrayed in Fig. 6. The engine parameters, including the nanoparticle quantity range of 20–100 ppm, were selected based on relevant literature [34–36] while the engine speed were based on studies discussed elsewhere [37,38].

Thirty experiments were conducted as a result of the experimental matrix of RSM. The performance indicators of diesel engines were evaluated to determine if the use of novel technology could improve efficiency without requiring any physical changes to the engine. Additionally, the emission parameters were recorded as environmental factors to be analyzed. Two readings were taken for

Table 5b
FAME composition of CNSOME.

Compound	Retention Time (min)	% Area (Concentration)
Methyl palmitate (C16:0)	~20.16	16.33 %
Methyl stearate (C18:0)	~23.35	8.72 %
Methyl oleate (C18:1)	~23.76	40.25 %
Methyl linoleate (C18:2)	~22.97	29.41 %
Methyl linolenate (C18:3)	~23.13	3.66 %

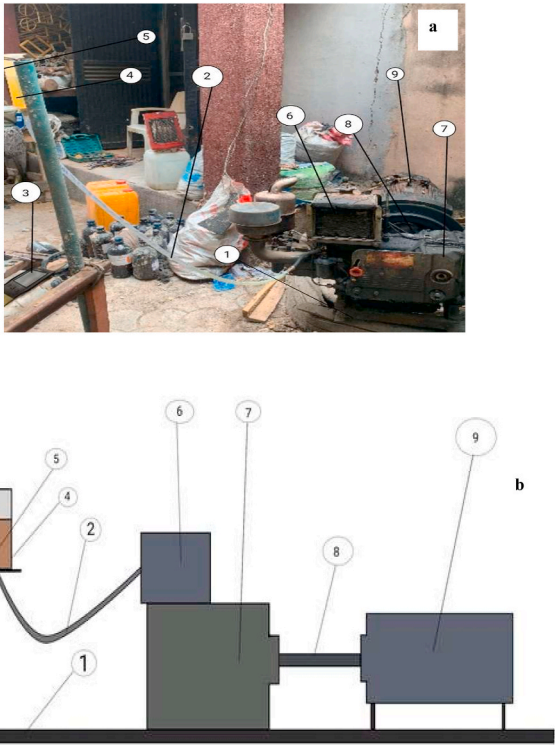


Fig. 6. Pictorial of the diesel engine set-up (a) (1) Machine bed, (2). Fuel hose, (3). Analyzer, (4). Diesel tank, (5). Biodiesel blend, (6). Injector and fuel pump unit, (7). Diesel engine, (8). Shaft, (9). Alternator (b) schematic representation.

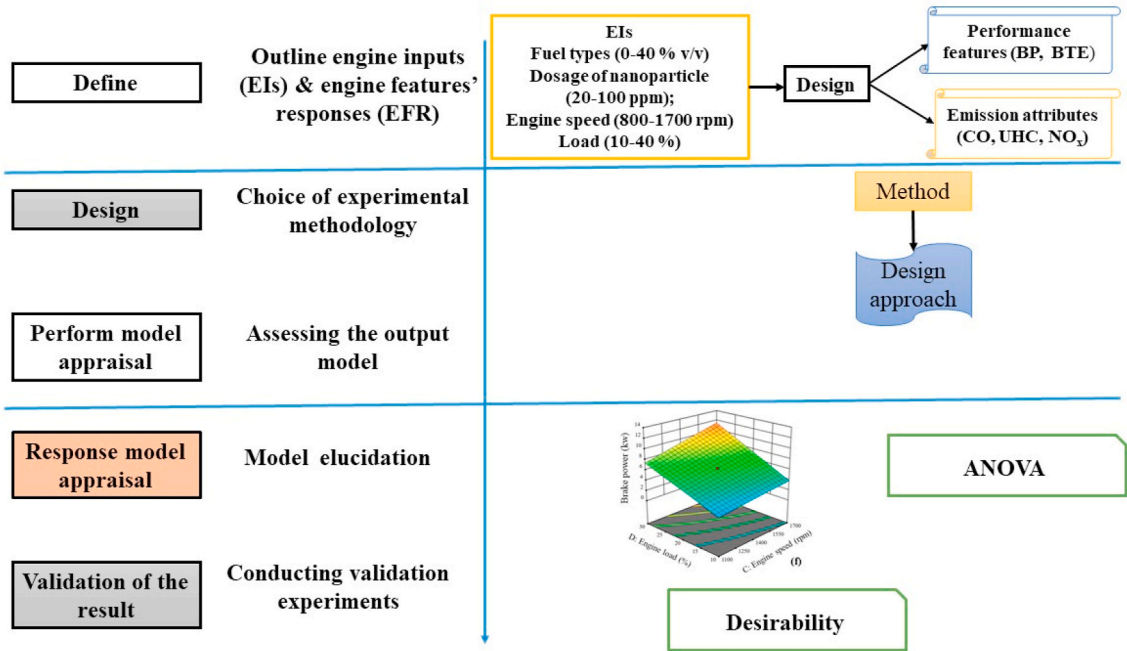


Fig. 7. Flow chart for engine feature and emission tails modelling.

each experimental run to ensure accuracy, and the average values were recorded. Fig. 7 illustrates the step-by-step process of the RSM modelling for engine tests.

2.4. Methodology for assessing diesel engine performance and exhaust emissions

The research assessed the performance characteristics of a direct injection (DI) single-cylinder diesel engine, including BP, BTE, and exhaust emissions features (EEFs) like CO, UHC, and NOx. The engine model utilized was a water-cooled, four-stroke, naturally aspirated test diesel engine (Zhejiang Sifang). The arrangement of the diesel engine connected to a hydraulic dynamometer is depicted in Fig. 6(a and b). The engine was test run to ensure that the accessories were in perfect condition. Before starting the measurements, the engine was warmed up for approximately 30 min using fossil diesel. The diesel fuel was then drained from the tank and replaced with the tested fuels. The measurements began when the lubricating oil temperature reached 90 °C. The engine load, speed, and fuel composition were examined, with variations ranging from 10 to 40 % load, 800–2000 rpm speed, and 0–40 vol% doped with nanoparticle dosage of 20–100 ppm. The engine parameters, such as the concentration of nanoparticles (ranging from 40 to 80 ppm) and the speed range, were determined based on existing research. Thirty experiments were carried out using an RSM experimental matrix. The performance of diesel engines was evaluated using specific indicators to determine the success of the new approach, without requiring any physical changes to the engines. Additionally, emission levels were monitored to assess the environmental impact of the approach. Two readings were taken for each experimental run to ensure precise measurements, and the average values were recorded. The flowchart illustrating the RSM modeling for engine tests is depicted in Fig. 7.

2.4.1. Uncertainty analysis

The errors and uncertainties in the experiments depend on factors such as instrument condition, calibration, environment, observation, and test planning [39]. Uncertainty analysis can demonstrate the accuracy of the experiments. Errors in the measured results are caused by errors in the parameters being measured. The estimated uncertainties for engine load, speed sensor, mass flow rate, and lower heating value are shown in Appendix 4 (Table A3). The uncertainties for Brake Power (BP) and Brake Thermal Efficiency (BTE) were calculated using Eqs. (A3) and (A4). Appendix 4 (Table A4) presents the estimated uncertainties for the emission characteristics. The total uncertainty assessment was conducted using Eq. (2) based on the principle of propagation of errors [40,41], and the results are summarized in Table 6.

$$\text{Aggregate uncertainty} = (\text{Uncertainty of BP})^2 (\text{Uncertainty of CO})^2 (\text{Uncertainty of NOx})^2 + (\text{Uncertainty of UHC})^2 \quad (2)$$

$$\text{Aggregate uncertainty} = \text{root} [(1.61365)^2 + (0.01832)^2 + (0.04641)^2] = 1.61442\% \text{ square}$$

$$\text{Aggregate uncertainty} = \text{square root} [(0.57822)^2 + (3.32787)^2 + (1.61365)^2 + (0.01832)^2 + (0.04641)^2] = 3.342\%$$

2.4.2. Optimization of a diesel engine using RSM and Rao algorithm

Fig. 8 illustrates the step-by-step process of conducting experimental modeling and optimization of a diesel engine using response surface modeling and the Rao algorithm. The experimental modeling and optimization of diesel engine emission and performance characteristics employ a framework that incorporates response surface modeling (central composite design) and the Rao-3 algorithm. This process is depicted in five sequential steps in Fig. 8. Step 1 entails recognizing the factors that can be optimized to enhance performance and emission characteristics. Step 2 specifies the conditions for optimization, including the number of individuals in the population and the number of iterations for the Rao-3 algorithm, as well as the parameters for central composite design, such as the blend type, nanoparticle concentration, engine speed, and engine load. Step 3 involved conducting experiments to gather data on various factors, including the type of blend used, the concentration of nanoparticles, the speed of the engine, and the load it was carrying. The output data: consisted of brake power, brake thermal efficiency, carbon monoxide, unburnt hydrocarbon, and nitrous oxide. This information was examined using a CCD matrix, and different graphs were created to comprehend the main effects and interactions. Equations based on empirical data were created to assist in predicting and optimizing outcomes.

In step 4, the parameters of the Rao 3 algorithm were fine-tuned to achieve the desired outcome by assessing the objective functions

Table 6
Uncertainty estimation of test engine.

S/N	Measured Quantity	Uncertainty
1.	Load (L)	0.8305
2.	Speed (N)	0.3899
3.	Mass flow rate (mf)	0.5275
4.	Lower heating value (LHV)	0.0408
5.	Brake power (BP)	0.9174
6.	Brake thermal efficiency (BTE)	1.0590
7	CO	3.38
8.	UHC	1.64
9.	NOx	0.67

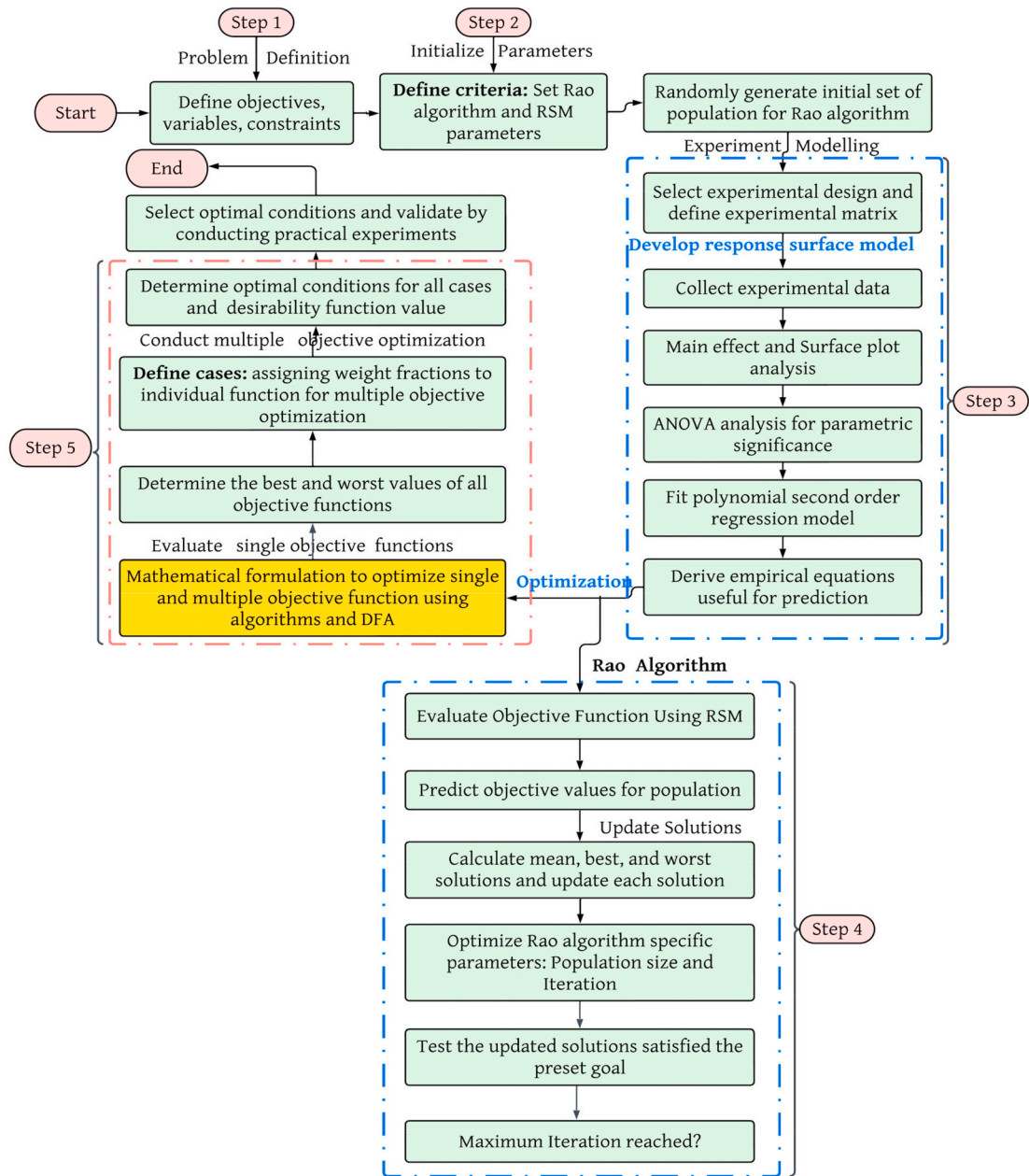


Fig. 8. Flow chart for optimizing a diesel engine using response surface modeling and the Rao algorithm.

for the best possible solutions. In step 5, the optimized Rao 3 parameters were utilized to determine the most and least favorable solutions, considering a single objective function. To achieve multiple objectives, the individual objective functions are combined using weight fractions and a desirability function approach. The composite desirability values were determined for various scenarios: case 1 with equal weight assigned to all five outputs, and cases 2–6 with the maximum weight fraction allocated to one output while keeping the others at low values. The highest composite desirability value obtained from the six case studies is suggested as the ideal condition. The best conditions were tested and proven to evaluate the effectiveness of the models and algorithms.

3. Results and discussion

3.1. Fuel properties and engine implications of ZnO-enhanced neem-castor biodiesel blends

Fig. 9a shows the variation of fuel density and viscosity with increasing ZnO nanoparticle dosage at room temperature. The trend

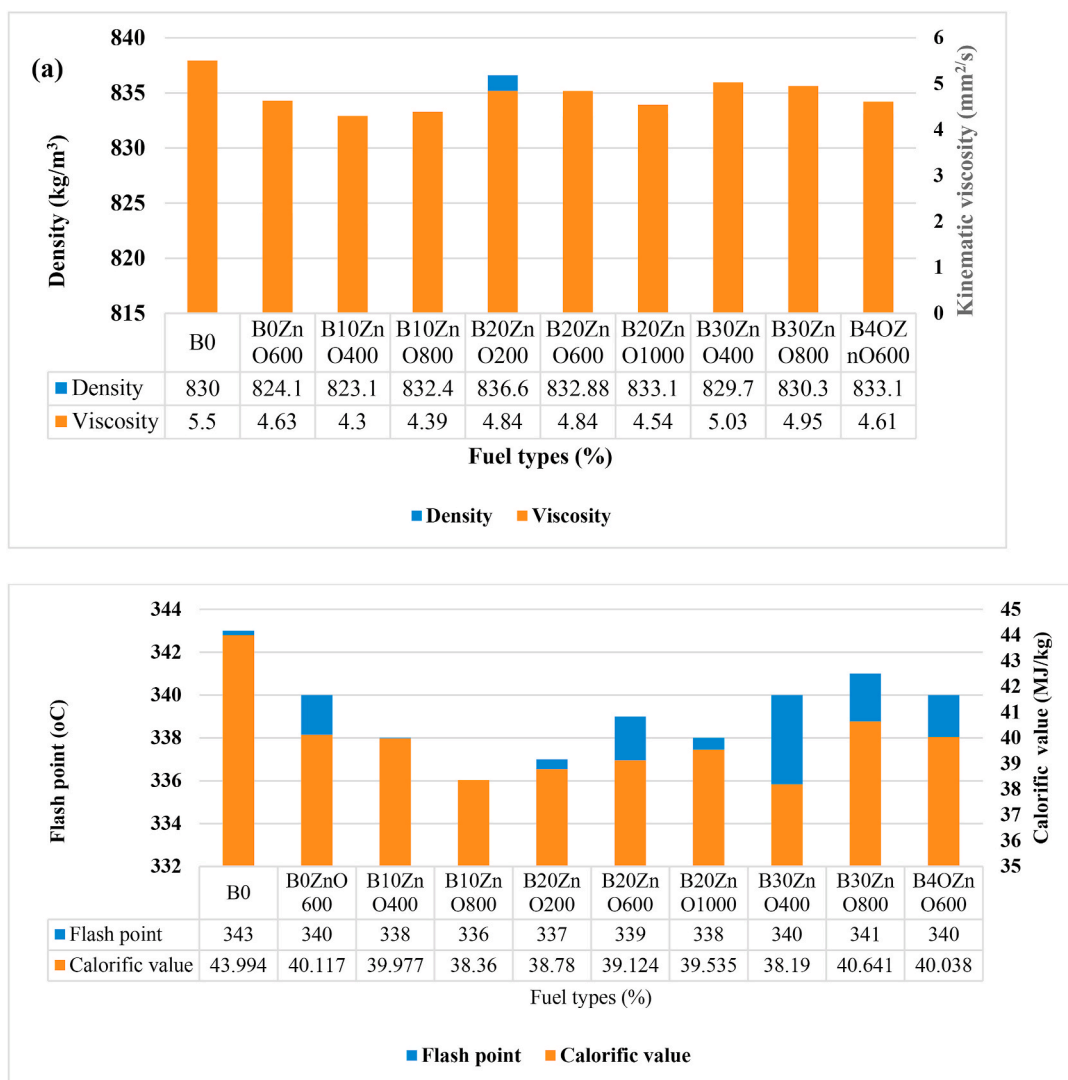


Fig. 9. Physicochemical properties of CNSOME/diesel/ZnO nanoparticle blends: (a) Density and viscosity, and (b) flash point and calorific value for different dosage levels of ZnO nanoparticles.

indicates a moderate increase in density and a slight rise in viscosity beyond 800 ppm, suggesting possible nanoparticle agglomeration that could affect atomization and combustion. The trend in fuel density and viscosity aligns with previous studies [42,43] where higher nanoparticle concentrations led to agglomeration and increased intermolecular interaction, resulting in elevated fuel viscosity and density. These changes are crucial for engine operation, as higher viscosity may hinder atomization and combustion efficiency, while increased density can impact fuel flow rate and injection timing. Therefore, determining the optimal nanoparticle dosage is essential to balance combustion efficiency with potential emissions and fuel handling issues.

Fig. 9b illustrates the variation in flash point and calorific value of ZnO-doped fuel blends with increasing nanoparticle dosage. The calorific value shows a slight upward trend, while the flash point increases up to 800 ppm and stabilizes thereafter. The trend in fuel in FP and CV of fuel concur elsewhere [44,45]. These trends indicate improved combustion potential and enhanced fuel safety, consistent with previous research. The increase in calorific value can be attributed to the catalytic activity of ZnO nanoparticles, promoting more complete combustion and higher energy content in the fuel blends. While a higher calorific value benefits engine performance by improving efficiency and reducing fuel consumption, the change observed in this study is modest, suggesting that ZnO nanoparticles enhance combustion without significantly altering the base fuel's energy content.

The rise in flash point with nanoparticle addition, especially up to 800 ppm, enhances fuel safety during handling and storage in high-temperature environments. The plateau in flash point beyond 800 ppm may be due to nanoparticle agglomeration, affecting their dispersion in the fuel matrix.

These findings have direct implications for engine operation and emissions, highlighting the importance of optimal nanoparticle dosing to maximize benefits while avoiding potential drawbacks [45].

3.2. Gathering of information

This section discusses the results of data collection based on the experimental matrices (i.e., CCD) and the derived regression equations that correlate the engine variables (fuel type, ZnO nanoparticle dosage, engine speed, load) with responses for diesel engine behavior (BP, BTE) and emission features (CO, UHC, and NOx). The effects of various engine parameters on multiple responses were also examined. The Rao algorithm was chosen to assess the objective functions for finding the most optimal solutions and to determine the best and worst solutions based on a single objective function. This was accomplished by finding the best and worst possible solutions through a process of iteration. CCD matrices were created for four engine variables, resulting in 30 experimental runs as shown in Table 7.

3.3. Diesel engine performance and emissions modelling

This research examined how different engine input parameters affected the performance of diesel engines (such as BP and BTE) and the emissions (such as CO, NOx, and UHC) using statistical regression models. The importance of these connections was established using p-values, and the ability of the models to predict outcomes was showcased through three-dimensional response surface plots.

3.3.1. Diesel engine efficiency

The performance of diesel engines running on a mixture of CNSOME-diesel blends was examined to determine their effectiveness, operability, and compatibility without any modifications to the engine. This study utilized a Design of Experiment (DOE) approach. These models were examined, evaluated and adjusted to meet the desired criteria of enhancing engine features such as BP and BTE. To evaluate the engine's performance and efficiency, two crucial factors, BP and BTE, were selected for inspection. Before utilizing these regression models (RMs) to forecast the performance characteristics, ANOVA was utilized to establish their correlation function with the engine inputs. The significance of parameters (linear: A, B, C, D; square: A², B², C² and D², 2-term interactions: AB, AC, AD, BC, BD, CD) are tested for the preset confidence level of 95 % (i.e. p-value <0.05). Parameters with p-values less than 0.05 are considered to have a statistically significant influence on BP and BTE. Table 8 presents the significant effects of factors on responses (BP and BTE), as indicated by their p-values. As evident from the analysis, the linear nanoparticle dosage and engine load, interaction parameter

Table 7
Experimentally designed matrix for diesel engine performance evaluation.

Exp. No.	Input variables				Outputs (Performance characteristics)		Outputs (Emission characteristics)		
	A: Fuel Blend (%)	B: Nanoparticle (ppm)	C: Engine speed (rpm)	D: Load (%)	BP (KW)	BTE (%)	CO (ppm)	UHC (ppm)	NOx (ppm)
1	30	80	1700	30	11.526	29.80	70	3.21	741
2	30	80	1700	10	3.8421	17.46	57	3.1	671
3	20	20	1400	20	7.2078	29.06	54	3.21	766
4	10	80	1700	30	11.526	32.15	71	3.3	727
5	20	60	800	20	3.6161	16.74	67	3.1	883
6	20	60	1400	20	6.3282	24.74	53	2.7	709
7	0	60	1400	20	6.3282	25.33	56	3.4	664
8	10	40	1700	30	11.526	36.57	75	3.1	775
9	20	60	1400	20	6.3282	24.74	53	2.7	709
10	40	60	1400	20	6.3282	24.17	53	3.2	716
11	10	80	1100	30	7.4582	27.06	60	3.19	681
12	30	40	1700	10	3.8421	20.93	56	3	902
13	30	40	1700	30	11.526	35.94	70	3.1	971
14	10	80	1100	10	2.4858	11.62	51	3.2	696
15	10	80	1700	10	3.8421	13.26	58	3.2	712
16	10	40	1700	10	3.8421	23.60	56	3	798
17	20	60	1400	20	6.3282	24.74	53	2.7	709
18	20	100	1400	20	6.3282	25.82	52	3.3	534
19	20	60	1400	20	6.3282	24.74	53	2.7	709
20	30	80	1100	10	2.4861	10.45	55	3	649
21	30	80	1100	30	7.4582	23.71	56	3	680
22	20	60	1400	40	12.526	32.82	71	2.8	723
23	20	60	1400	20	6.3282	24.74	53	2.7	709
24	20	60	2000	20	9.0402	31.64	76	3.2	1049
25	10	40	1100	10	2.4861	13.57	56	3.25	767
26	30	40	1100	30	7.4582	24.44	66	3.1	861
27	10	40	1100	30	7.4582	26.87	71	3.1	735
28	20	60	1400	20	6.3282	24.74	53	2.7	709
29	20	60	1400	0	0	0.00	46	2.8	742
30	30	40	1100	10	2.4861	14.43	53	3	827

BP=Brake power; BTE = Brake thermal efficiency; CO =Carbon monoxide; UHC = Unburnt hydrocarbon; NOx = Nitrous oxide.

Table 8
P-values of the terms in the diesel engine performance (DEP) model.

Factors	BP	BTE
A	0.9996	0.1814
B	0.0041	0.0001
C	0.1829	0.0001
D	0.0054	0.0001
AB	0.9996	0.7071
AC	0.9996	0.4318
AD	0.9996	0.1028
BC	0.9996	0.0071
BD	0.9996	0.1533
CD	< 0.0001	0.2292
A ²	0.5778	0.7355
B ²	0.0037	0.0522
C ²	0.5775	0.4061
D ²	0.2632	0.0001

Significant- ($0.000 < p \leq 0.05$)

(A: Fuel types/blends, B: Nanoparticle's dosage, C: Engine speed, D: Load, AB: Fuel types x nanoparticle's dosage, AC: Fuel types x engine speed, AD: fuel type x load, BC: Nanoparticle's dosage x engine speed, BD: Nanoparticle's dosage x load, CD: Engine speed x Load, A²: Quadratic of fuel types, B²: Quadratic of nanoparticle's dosage, C²: Quadratic of engine speed, D²: Quadratic of load).

representing engine speed and load, and the quadratic of nanoparticle dosage are the most influential factors in the BP model. The linear nanoparticle dosage, engine speed, engine load and quadratic of engine load have practical importance in the BTE model. The performance characteristics of different IC engines can be assessed using Table 9 that lists the regression equation items. Eqs. (3a)-(3b) can appropriately theorize BP and BTE.

The coefficient of determination (R^2) is used to explain how well the independent variables of a model explain the variability of the dependent variable. Note that, the R^2 (all terms) and adj. R^2 (excluding insignificant terms) values for the developed models are found to be equal to 0.9989 and 0.9979 for BP, and 0.9838 and 0.9686 for BTE, respectively. A higher R^2 value signifies that the developed BP and BTE regression equations, acquired from experimental input-output data through engine tests, are statistically adequate for making accurate predictions and optimizing the engine test conditions with less variation. Fig. 10a and b present scatter plots that graphically support the higher R^2 and adjusted R^2 values obtained for BP and BTE. The data points show good agreement between experimental and predicted values, close to the ideal line, confirming the statistical validity, accuracy, and robustness of the developed models. Therefore, these models are best suited to optimize engine test conditions with minimal error.

3.3.2. Emission characteristics

Emission attributes of vehicular diesel engines operated by CNSOME/diesel blends were evaluated for environmental benign using the DOE. These models were assessed, appraised and optimized for the desired criteria of abating environmental topographies namely CO, NO_x, and UHC. To scrutinize the eco-friendly features, three key parameters—CO, NO_x, and UHC—were selected. Prior to adopting these RMs to estimate emission features, ANOVA was adopted to prove their relationship function with the inputs or control factors. Table 10 presents the substantial influence of factors on responses (CO, NO_x, and UHC) based on p-values. The effect of linear terms (fuel types, nanoparticle dosage, engine speed, and engine load), quadratic terms (engine speed, and engine load) and interaction terms (fuel types x engine load, nanoparticle dosage x engine speed, nanoparticle dosage x engine load and engine load x engine speed) influenced the CO model. The UHC model is significantly controlled by the linear terms (fuel types, nanoparticle dosage and engine speed), interaction terms (fuel types x nanoparticle's dosage, fuel types x engine load) and quadratic terms (nanoparticle dosage and engine speed). NO_x is influenced by all linear and square terms and interaction terms (excluding fuel types x engine load, and nanoparticle dosage x engine load). The emissions of various IC engines can be evaluated using the regression equation itemized in Table 11. Eqs. (4a) -(5c) can appropriately postulate CO, NO_x, and UHC.

The term R^2 and adj. R^2 values for the developed models were found to be equal to 0.9767 and 0.955 for CO, 0.9877 and 0.9762 for UHC, and 0.9841 and 0.9693 for NO_x, respectively. All three models developed for emission characteristics (CO, NO_x and UHC) produced better R^2 value depicting that the models are statistically adequate. Fig. 11a–c presents scatter plot where the experimental and model predicted data points were close to the ideal trend line depicting that the models were statistically adequate and predicted with minimal deviation.

3.3.3. Impact of control variables on BP

The 3Ds for the BP with blend type and nanoparticle dosage, blend type and engine speed, blend type and engine load, nanoparticle dosage and engine speed, nanoparticle dosage and engine load, engine speed and engine load are depicted in Fig. 12(a–f).

As depicted in Fig. 12a, there is no significant variation in the BP of diesel engines when using different blend types with ZnO nanoparticles. The addition of nanoparticles does not have a substantial impact on BP, which could be due to the lower energy content

Table 9
Regression equations for DEP.

Regression equations for DEP	
BP	$0.559543 + 0.006259A - 0.03197B + 0.000487C + 0.011719D - 0.0000000375AB - 0.0000000625AC - 0.00000001875AD + 0.00000003125BC + 0.00000009375BD + 0.00022CD + 0.000156A^2 + 0.00023581B^2 - 0.000000173762C^2 - 0.000319D^2$ (3a)
BTE	$-17.68021 - 0.055167A - 0.0579B + 0.025679C + 1.36142D + 0.00069AB + 0.000097AC - 0.006237AD - 0.00019BC + 0.0027BD + 0.00015CD - 0.000944A^2 + 0.0014B^2 - 0.000026C^2 - 0.00015D^2$ (3b)

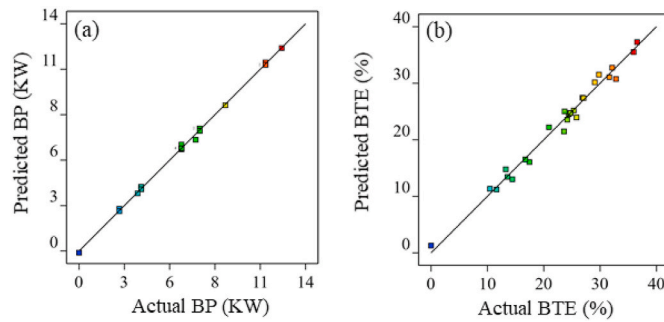


Fig. 10. Predicted versus actual values for engine performance parameters: (a) Brake Power in kW, and (b) Brake Thermal Efficiency in %.

Table 10

P-values of the terms in the emission features (EPs) model.

Factors	CO	UHC	NOx
A	0.0278	0.0001	0.0001
B	0.0043	0.0001	0.0004
C	0.0001	0.0001	0.0371
D	0.0001	0.2218	0.0471
AB	0.1388	0.0001	0.0246
AC	0.8889	0.0770	0.0246
AD	0.05	0.0024	0.0589
BC	0.0052	0.1393	0.0001
BD	0.0029	0.4675	0.7103
CD	0.0093	0.1328	0.0029
A ²	0.0553	0.2200	0.0001
B ²	0.3516	0.0007	0.0001
C ²	0.0001	0.0001	0.0001
D ²	0.0001	0.0840	0.0022

of CNSOME [46].

Fig. 12b illustrates the variation of BP with engine speed and different fuel blends. As noted, even though BP does not show a significant change with the increase in the fuel types, BP increases with the variation in the engine speed (ES) for all fuel types and reduces at an optimal range of the ES. The decrease in BP at the ES is believed to be caused by a decrease in the volumetric efficiency. The impact of engine load and fuel type on BP is illustrated in Fig. 12c. The BP rises with the engine load for all blends, but there is only a very small change when the fuel type is altered. These findings are consistent with the results obtained by Shirmeshan et al. [47] and Jindal et al. [48]. Similar to Fig. 12d, BP is improved with the addition of nanoparticles and engine speed. This finding is supported by the results reported by El-Seesy et al. [49].

The increase in BP is influenced by the interaction between the ES and nanoparticle [50]. As depicted in Fig. 12e, higher loads and increased ZnO nanoparticle dosages result in the progression of BP. When the nanoparticles were subjected to higher loads and operated under optimal conditions, the maximum BP was attained [51,52]. The combination of increased engine load and speed resulted in the highest BP, as depicted in Fig. 12f. This might be due to the increased temperature in the engine combustion chamber as a result of a better air-fuel mixture and complete combustion [53].

3.3.4. BTE model

Surface plot analysis investigates the impact of two variable interactions while keeping the rest of the factors constant at fixed mid-values on BTE (Fig. 13a–f). All surface plots appear to exhibit a consistent upward trend (linear behaviour), with the exception of the interaction between engine speed and nanoparticle concentration (BC).

Surface plot analysis investigates the impact of two variable interactions, while keeping the rest of the factors constant at fixed mid-values, on BTE (Fig. 13a–f). All surface plots appear to exhibit a consistent upward trend (linear behaviour), with the exception of the interaction between engine speed and nanoparticle concentration (BC). As the biodiesel content increases, there is a slight decrease in the BTE (Fig. 13a, b, and c). This occurs because the fuel properties of biodiesel, such as a higher cetane number resulting in a shorter delay time, lower calorific value, and high viscosity causing poor atomization in the engine cylinder, differ with changes in biodiesel content. The increased biodiesel content in the blended fuel led to a slightly lower BTE [54]. The concentration of ZnO nanoparticles increases with the magnitude of BTE present (refer to Fig. 13a–d–e). This improvement can be attributed to the high surface-area-to-volume ratio of nanoparticles, which enhances catalytic activity and promotes micro-explosions of fuel droplets. This results in better atomization, improved air–fuel mixing, and more complete combustion [55,56]. As the biodiesel content decreases and the engine load and speed increase (as shown in Fig. 13b, c, and f), the proportion of BTE also increases. The pressure within the engine cylinder and the temperature of the combustion gas rise, leading to an increase in power output [57]. The highest BTE was

Table 11
Regression equations for EFs.

Regression equations for emission profile	
CO	$178.07755 - 0.4145834A - 0.40512B - 0.168727C - 0.022917D + 0.003441AB - 0.000021AC - 0.00938AD + 0.00024BC - 0.0078BD + 0.000438CD + 0.006979A^2 + 0.000807B^2 + 0.000055C^2 + 0.000438D^2$ (4a)
NOx	$1915.698 + 7.22708A + 5.88229B - 1.94368C - 9.57708D - 0.17531AB + 0.002812AC + 0.161875AD - 0.00116BC + 0.01656BD + 0.002354CD - 0.043437A^2 - 0.0359B^2 + 0.000718C^2 + 0.0062813D^2$ (4b)
UHC	$8.02564 - 0.074729A - 0.04759B + 0.004196C - 0.02585D + 0.000103AB + 0.000009375AC + 0.000169AD + 0.0000069791BC + 0.000015625BD + 0.000009791CD + 0.001482A^2 + 0.00034244B^2 + 0.00000123032C^2 + 0.000232D^2$ (4c)

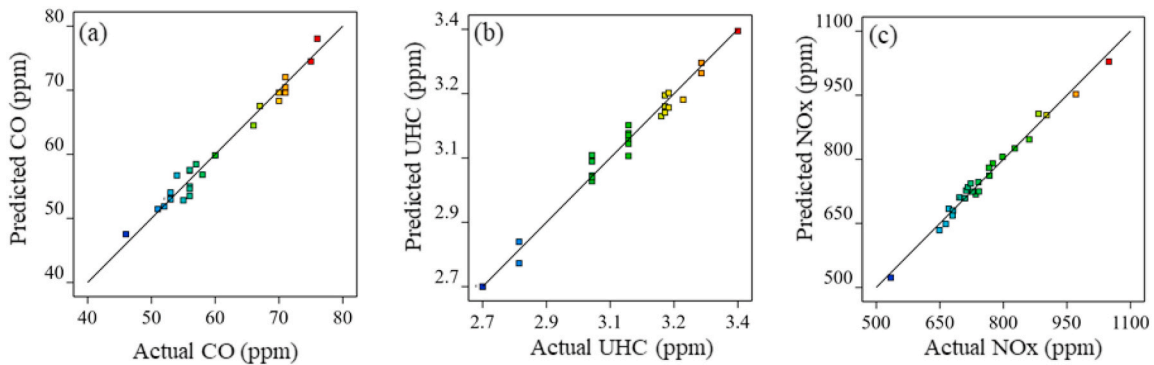


Fig. 11. Predicted versus actual values for engine emission parameters: (a) CO in ppm, (b) UHC in ppm, and (c) NOx in ppm.

achieved when both the engine load and speed were at their highest values, as shown in Fig. 13f.

3.3.5. CO model

The surface plots in Fig. 14a–f are used to demonstrate the impact of various factors on CO emissions. The combined influence of blend type and nanoparticle concentration was found to have a negligible effect on CO emissions (refer to Fig. 14a). The decrease in CO emissions is credited to the combination of the nanoparticle dosage and CNSOME, resulting in improved combustion. These findings are consistent with the research conducted by Rizwanul et al. [58]. The interaction between engine speed (a significant factor) and blend type (a minor contributor) led to a decrease CO emissions. Biodiesel contains oxygen atoms that promote more thorough combustion, while nanoparticles act as combustion catalysts, speeding up oxidation and improving the air-fuel mixture—thereby decreasing CO emissions (refer to Fig. 14b). Soudagar et al. [59] found that the combination of engine speed and the use of oxygenated fuels led to a reduction in CO emissions. Fig. 14c shows how the combined impact of engine load and blend type affects the emission levels. When vehicles carry heavier loads and travel at higher speeds, the combustion process becomes less efficient, resulting in reduced mixing time and increased fuel consumption, which in turn leads to higher levels of CO emissions (refer to Fig. 14c). Agarwal et al. [60] suggested that higher levels of CO emission are caused by incomplete combustion, which occurs when there is not enough oxygen in the combustion chamber. A similar observation was reported by Hasan and Rahman [61]. The relationship between nanoparticle dosage and CO emissions is shown in Fig. 14d. As the quantity of nanoparticles and load increases, there is a decrease in CO emissions. This decrease is attributed to the improved combustion efficiency due to the thermal conductivity of CNSOME doped with ZnO nanoparticles [51]. Furthermore, a decrease in CO emissions is associated with better combustion due to improved mixing and a shorter ignition delay [62,63]. Fig. 14e shows a significant decrease in CO emissions as the amount of nanoparticles increases and the ES rises. The combined effect of higher ES and the enhancement of thermal conductivity in CNSOME doped with ZnO nanoparticles result in improved combustion, which in turn leads to a decrease in CO emission [62]. Similar to Fig. 14f, the interface between speed and load demonstrates CO emissions tend to decrease as engine speed increases but increase as engine loads rise. The combination of high speeds and high loads has a substantial impact on CO emissions.

3.3.6. NOx model

The behaviour of four factors can be easily seen in the surface plots drawn for NOx, as shown in Fig. 15(a–f). NOx emissions are depicted with various impacts of factors. The higher concentration of biodiesel blends resulted in a slight increase in NOx emissions, as shown in Fig. 15a–c. The marginal increase in NOx emissions caused by biodiesel might be due to the initial temperature required to match the ignition time, making it challenging to increase the oxygen in the fuel, which promotes the combustion phenomenon with increased combustion temperature and NOx emissions [64,65]. The higher concentration of nanoparticles had a positive impact, resulting in reduced NOx emissions (see Fig. 15a–d, and e). This is because the nanoparticles reduce the ignition time, possibly due to a catalytic effect during combustion [66]. As engine speed and load increase, higher levels of NOx emissions are detected (see Fig. 15f). This occurs because more fuel is supplied, leading to poor vaporization, a longer delay period, insufficient combustion, and resulting in higher values of NOx emissions [67].

3.3.7. UHC model

Three-dimensional surface plots were created to investigate the impact of input variables (blend type, nanoparticle, engine speed, and engine load) on the response behaviour of the output (UHC) (see to Fig. 16a–f).

All the plots indicated that the inputs did not exhibit a linear relationship with the output. When the volume percentage of biodiesel in the blended fuel was increased, there was a significant decrease in UHC levels, reaching up to 20 vol %, with minimal change remained minimal in the output variable (see Fig. 16a–c). Mixing biodiesel with other types of fuel, such as diesel, enhances the fuel's physical characteristics, engine performance, and reduces harmful emissions [68].

Higher concentrations of nanoparticle initially reduced UHC emissions, but further increases did not have a significant impact. Adding nanoparticles to biodiesel can help decrease nitrogen oxide levels, air oxidation, and issues related to incomplete combustion issues [69,70].

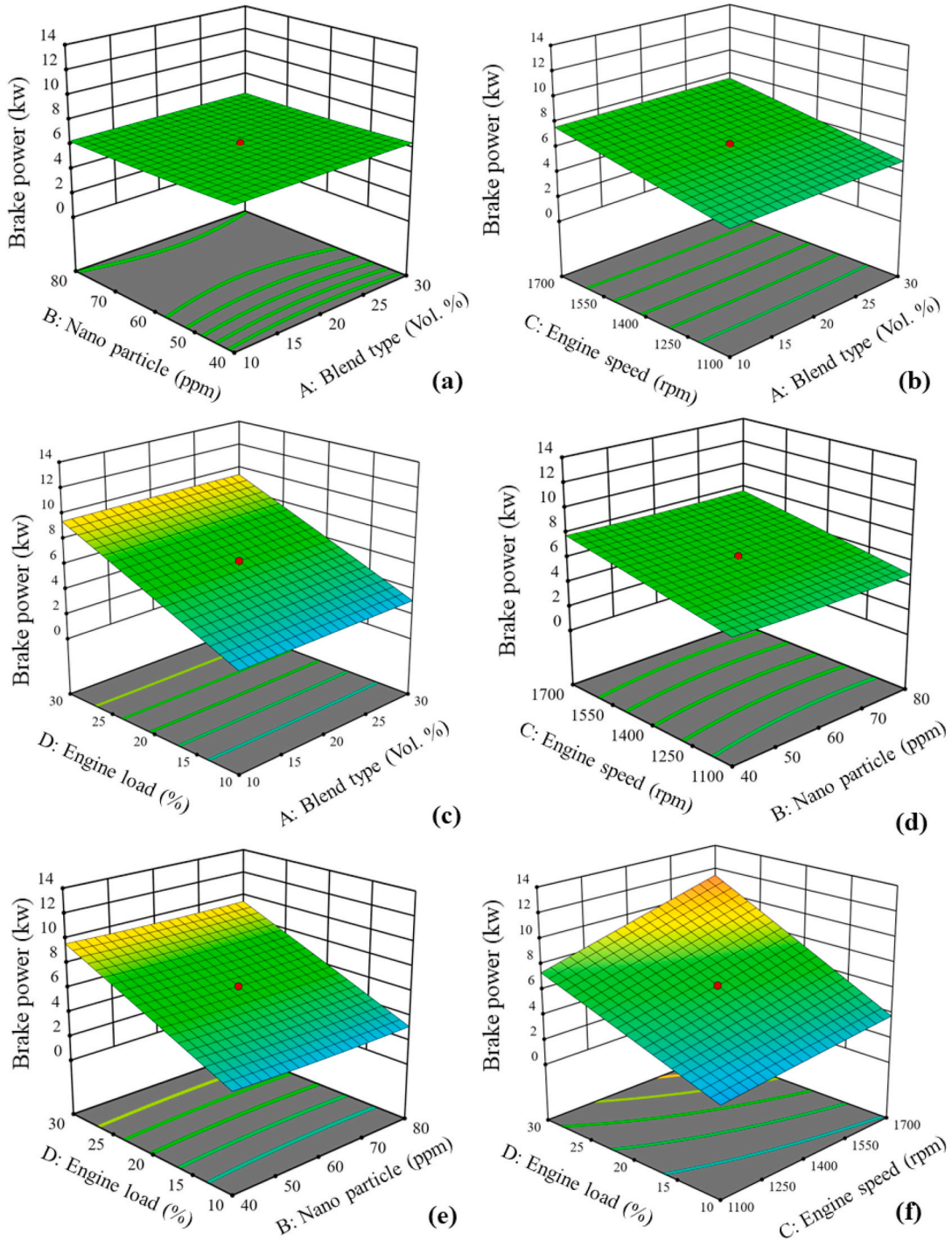


Fig. 12. Surface plots for BP with: (a) blend type and nanoparticle, (b) blend type and engine speed, (c) blend type and engine load, (d) nanoparticle and engine speed, (e) nanoparticle and engine load, f) engine speed and engine load.

As engine speed and load increased up to the mid-range, UHC levels decreased (see Fig. 16f). This is because increasing engine speed and load result in a more uniform distribution of air and fuel, improving combustion efficiency as the temperature rises. However, as engine speed and load contribute to increase, UHC emissions also rise, possibly due to more fuel being injected at higher engine loads and speeds, leading to a higher risk of incomplete combustion due to reduced oxygen content [71].

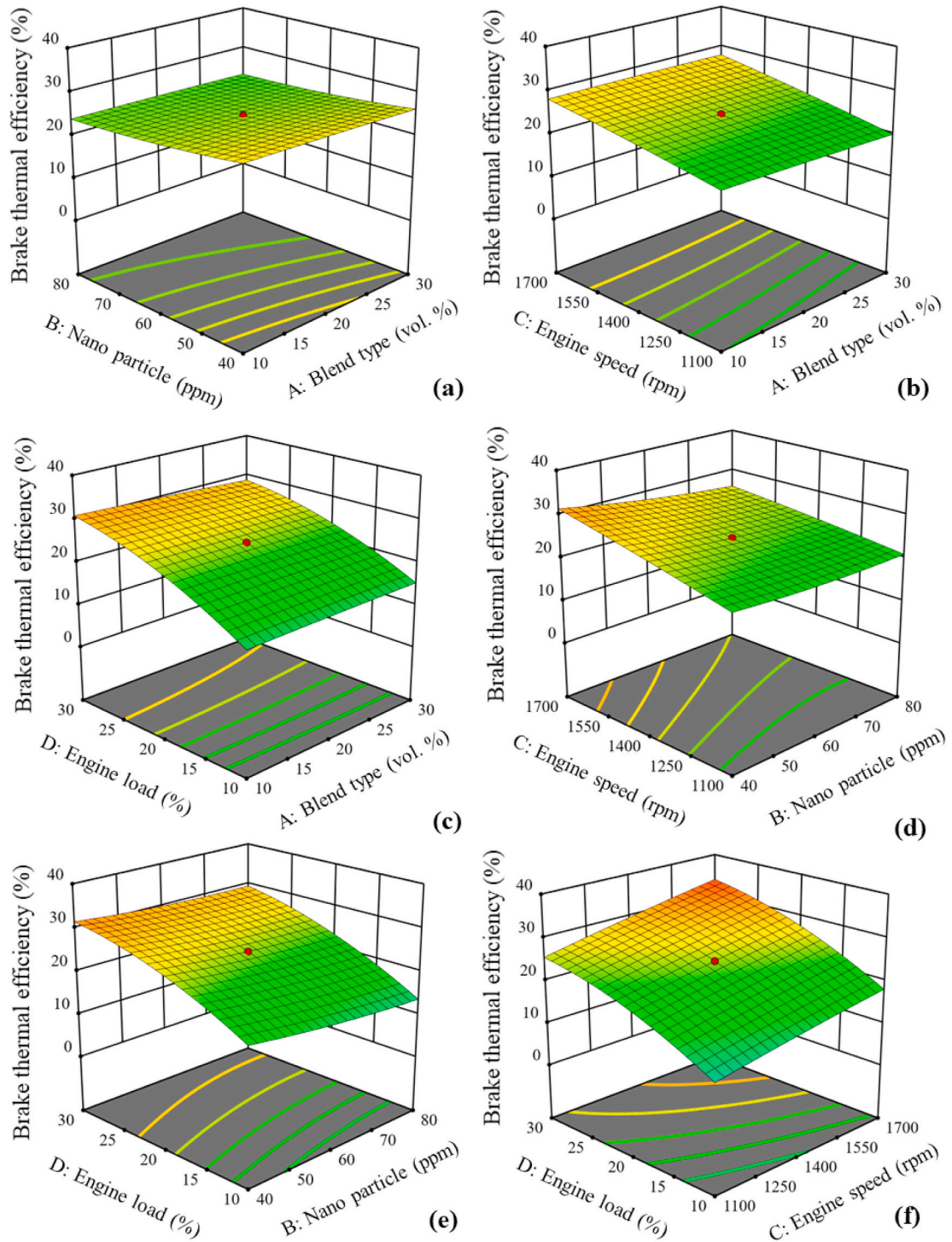


Fig. 13. Surface plots for BTE with: (a) blend type and nanoparticle, (b) blend type and engine speed, (c) blend type and engine load, (d) nanoparticle and engine speed, (e) nanoparticle and engine load, (f) engine speed and engine load.

3.4. Optimization using Rao algorithm

Rao suggested three population-based algorithms that did not rely on metaphors, namely Rao-1, Rao-2, and Rao-3 [72]. These algorithms are straightforward, simple to implement, and can be used with a mechanism that explores and exploits the search region, iterating the best solution, worst solution, and random interactions between the population [30,31]. Unlike other popular

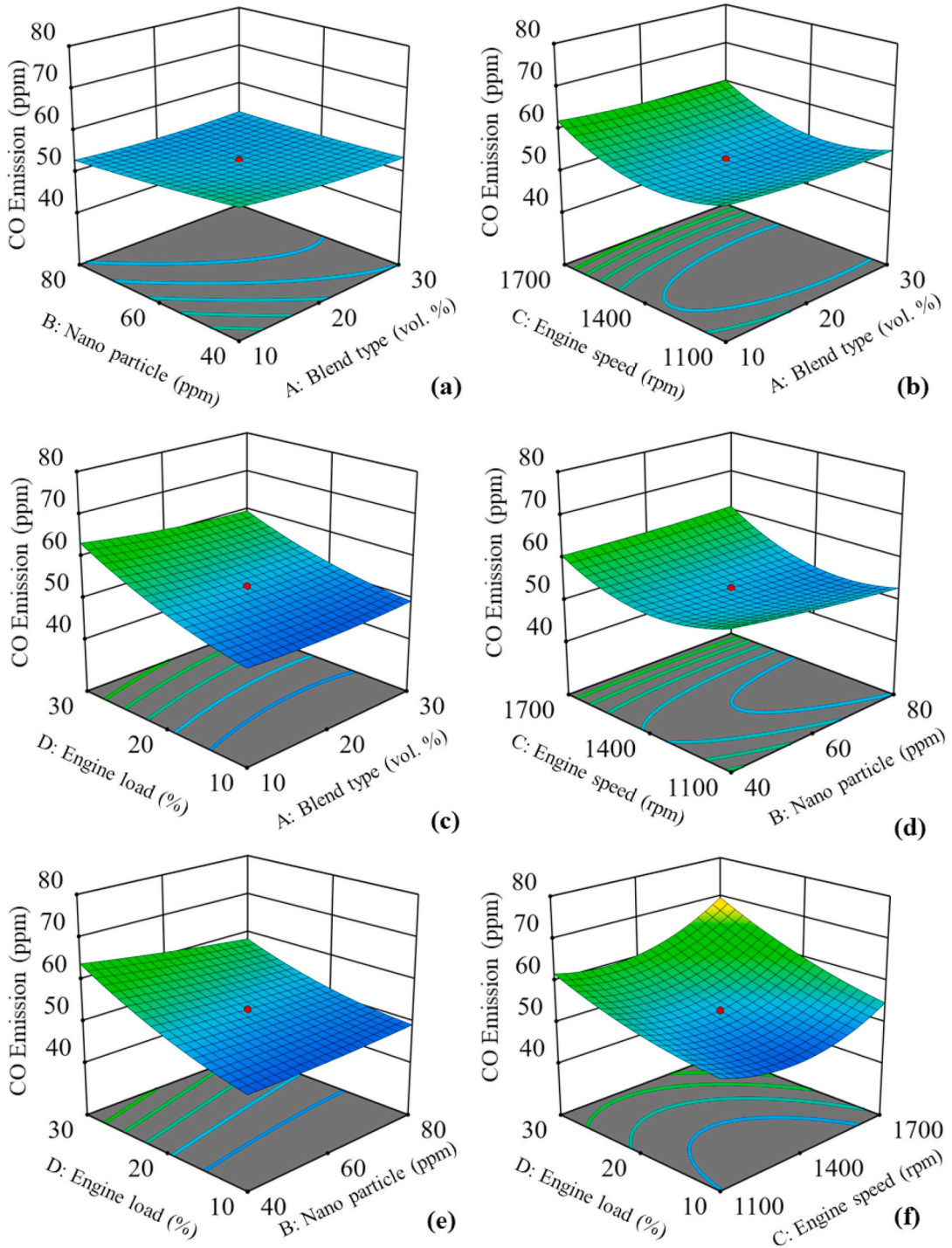


Fig. 14. Surface plots for CO Emission with: (a) blend type and nanoparticle, (b) blend type and engine speed, (c) blend type and engine load, (d) nanoparticle and engine speed, (e) nanoparticle and engine load, (f) engine speed and engine load.

population-based algorithms (like Genetic Algorithm: GA, Bald Eagle Search, Teacher Learner based Optimization: TLBO, Grey Wolf Optimization, Particle Swarm Optimization: PSO, JAYA), Rao algorithms do not require tuning algorithm specific parameters and do not trap much in local minima solutions [72–75]. The performance of Rao algorithm showed superiority over other algorithms (such as PSO, GA, TLBO, Ant Colony Optimization, Big-Bang and Big Crunch algorithm, JAYA) for optimizing construction scheduling problems [76], turbocharged DI diesel engine [77], turning process [78], fused deposition modeling process [75], and so on. Rao

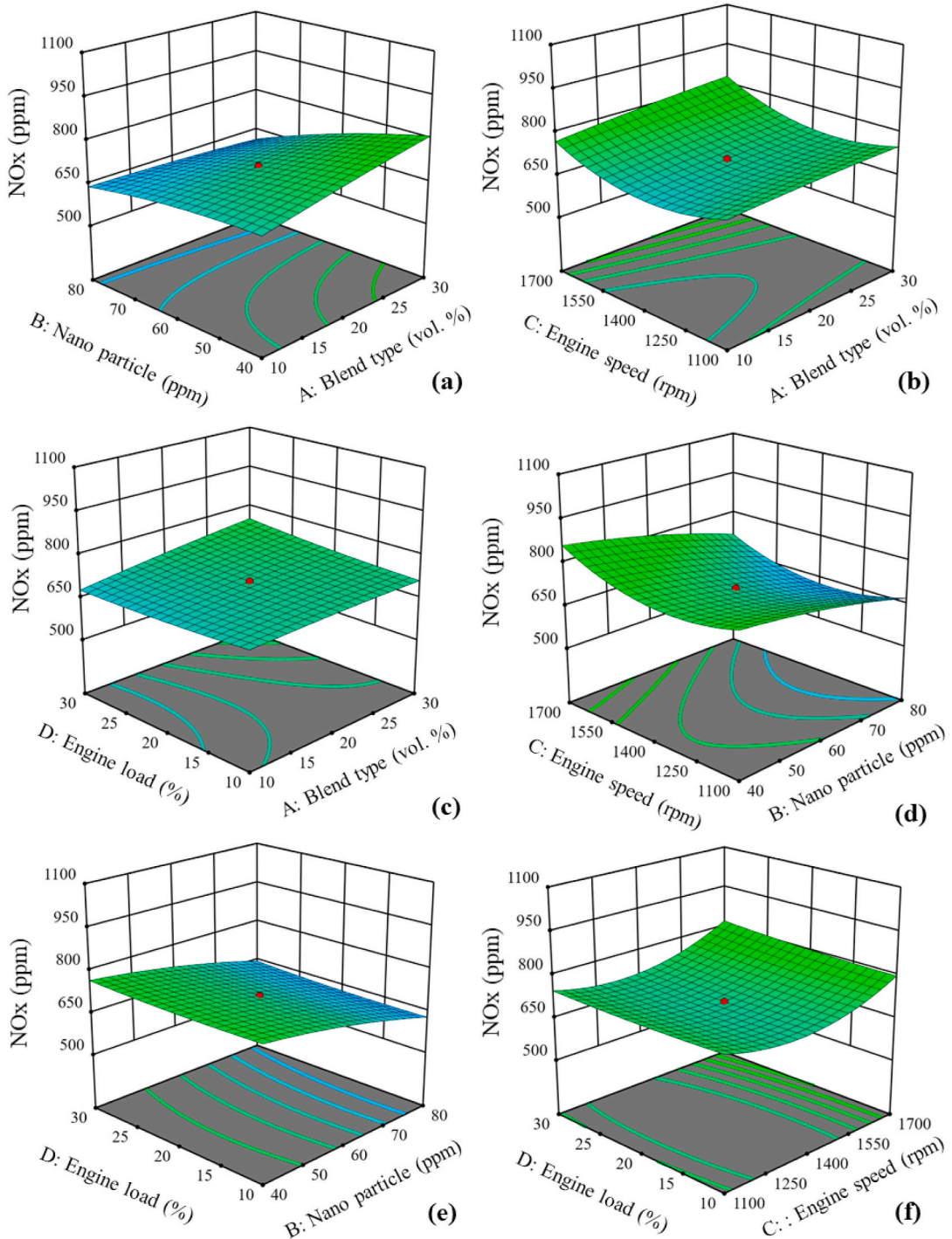


Fig. 15. Surface plots for NOx with: (a) blend type and nanoparticle, (b) blend type and engine speed, (c) blend type and engine load, (d) nanoparticle and engine speed, (e) nanoparticle and engine load, (f) engine speed and engine load.

algorithms (Rao-3) showed computational competence than GA, JAYA, PSO, Rao-1 and Rao-2 algorithms in optimizing the milling process [27,75]. The Rao-3 algorithm's superiority prompted us to undertake an optimizing task that simultaneously optimizes the performance and emission characteristics of a diesel engine. The step-by-step process of working with mathematical equations is detailed in published literature [30,31,72]. The framework employed to conduct optimization is illustrated in Fig. 8. The outcomes of single-objective and multiple-objective optimization, achieved through the application of the Rao-3 algorithm, are presented in Table 12.

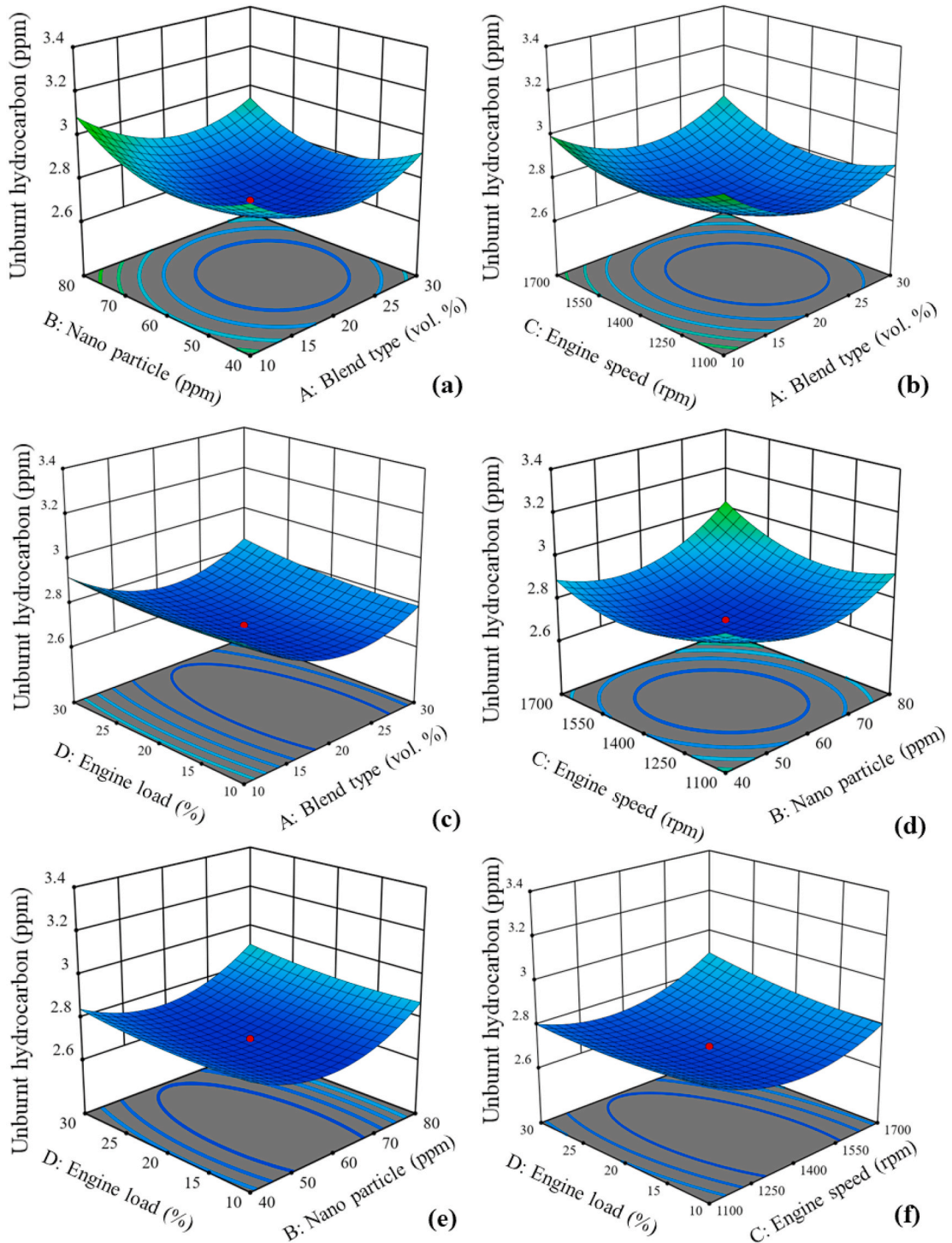


Fig. 16. Surface plots for UHC with: (a) blend type and nanoparticle, (b) blend type and engine speed, (c) blend type and engine load, (d) nanoparticle and engine speed, (e) nanoparticle and engine load, (f) engine speed and engine load.

3.4.1. Single and multi-objective optimization

The Rao-3 algorithm is applied to minimize the emissions (UHC, NO_x, CO) and maximize the performance (BP and BTE) while optimizing parameters (nanoparticle, blend type, engine speed and engine load) associated with diesel engines. The Matlab 17 software platform was utilized to enhance engine performance and emission characteristics in diesel engines. There are five outputs that contradict each other (i.e., both aim to maximize and minimize) that need to be optimized. The Rao-3 algorithm is applied to solve the

Table 12

Summary of results of single objective optimized conditions for the biodiesel process.

Optimization technique	Objective type	Input variables				Output value	Experimental value
		A: Blend type (Vol. %)	B: nanoparticle (ppm)	C: Engine speed (rpm)	D: Engine load (%)		
Rao-3	Maximize BP	20	40	1700	30	11.57 Kw	11.9 Kw
DFA		20	40	1700	30	11.57 Kw	
Rao-3	Maximize BTE	10	40	1700	30	38.52 %	37.47 %
DFA		10	40	1700	30	38.52 %	
Rao-3	Minimize CO	10	80	1318	10	52.67 ppm	54.3 ppm
DFA		24.5	40	1403	10	58.25 ppm	
Rao-3	Minimize NOx	30	80	1340	10	590.8 ppm	603.4 ppm
DFA		30	80	1342	10	590.8 ppm	
Rao-3	Minimize UHC	21.9	58	1397.8	15.4	2.64 ppm	2.55 ppm
DFA		23.64	58.33	1377.65	13.38	2.65 ppm	

derived empirical regression equations (Eqs. (3a), (3b) and (4a), 4b and 4c) to conduct an optimal search subject to input variable constraints for both single and multiple-objective optimization tasks.

Input Variable Constraints:

$$\begin{aligned}
 10 &\leq \text{Fuel blend or Blend type (A)} \leq 30 \\
 40 &\leq \text{Nanoparticle Concentration (B)} \leq 80 \\
 1100 &\leq \text{Engine speed (C)} \leq 1700 \\
 10 &\leq \text{Engine load (D)} \leq 30
 \end{aligned}$$

3.4.1.1. Results of single objective optimization. A single objective optimization task is carried out to determine the optimal conditions for an individual response by applying the Rao-3 algorithm and DFA. Although the Rao-3 algorithm is a parameter-free optimization technique, the performances are influenced by common algorithm parameters such as population size and maximum iterations. Smaller population sizes ensure faster convergence but might result in premature convergence due to limited diversity. However, larger populations enhance the exploration capabilities but might increase computation time. Few iterations may not capture complex non-linear behaviour to locate global minima, whereas maximum iterations might not reach the potential solutions. Therefore, a parametric study has been conducted by varying population size between 10 and 100 and iterations from 10 to 100. Initially, the population size is varied between 10 and 100 (after keeping the iterations fixed at 50) and the output values are recorded. The maximum output value corresponding to a population size of 30 was considered optimal and tested for iterations varying between 10 and 100. The resulting optimal parametric conditions that maximize the output value correspond to the population size and maximum iteration maintained at 30 and 40, respectively. The optimal conditions determined for all the individual responses (maximum values of BP and BTE and minimum values of CO, NOx, and UHC) using the DFA and Rao-3 algorithm are presented in Table 12. The Rao-3 algorithm performed marginally better than DFA in optimizing all individual responses.

Experiments were carried out to assess the effectiveness of the Rao-3 algorithm in identifying the optimal parametric conditions. It was observed that the BP peaked at 11.9 kW when the fuel blend type was set at 20 % vol., with a lower nanoparticle concentration, higher engine speed, and engine load (refer to Table 12). To achieve the highest possible value of BTE at 37.47 %, the engine speed and load should be set at 1700 rpm and 30 %, while using 40 ppm of nanoparticle and 10 vol% of biodiesel in the diesel fuel. When the engine operated at a load of 10 % and a speed of around 1318 rpm, CO emissions were measured at 54.3 ppm, while NOx emissions were recorded at 603.4 ppm. Low values of UHC i.e., 2.55 ppm, resulted from the parametric condition i.e., 21.9 vol% of blend type, 58 ppm of nanoparticle, 1397.8 rpm of engine speed and 15.4 % of engine load, respectively. The computed percent error ($100 \times (\text{experimental value} - \text{predicted value}) / \text{predicted value}$) is found to be equal to 2.77 % for BP, 2.8 % for BTE, 3 % for CO, 2.09 % for NOx, and 3.53 % for UHC emission, respectively.

3.4.1.2. Results of multiple objective optimization. Table 12 presents the different optimal conditions for individual output. It is important to note that when dealing with multiple objectives that have conflicting requirements, there are numerous potential solutions that can evolve, and these solutions can vary significantly from one another. Achieving a balance between conflicting requirements to produce a single parametric condition necessitates the use of appropriate mathematical formulation to perform multiple objective optimization [74,79,80]. The mathematical model was developed with the objective of maximizing the overall objective function (minimize: UHC, NOx, and CO, and maximize: BP and BTE) utilizing desirability function approach (DFA) presented in Eq. (5).

$$DFA_{\text{Composite}} = \sqrt[5]{(DFA_{BP}^{W_1} \times DFA_{BTE}^{W_2} \times DFA_{CO}^{W_3} \times DFA_{UHC}^{W_4} \times DFA_{NOx}^{W_5})} \quad (5)$$

$$DFA_{BP} = \frac{BP - BP_{\min}}{BP_{\max} - BP_{\min}} \quad (6)$$

$$DFA_{BTE} = \frac{BTE - BTE_{\min}}{BTE_{\max} - BTE_{\min}} \quad (7)$$

$$DFA_{CO} = \frac{CO_{\max} - CO}{CO_{\max} - CO_{\min}} \quad (8)$$

$$DFA_{UHC} = \frac{UHC_{\max} - UHC}{UHC_{\max} - UHC_{\min}} \quad (9)$$

$$DFA_{NOx} = \frac{NOx_{\max} - NOx}{NOx_{\max} - NOx_{\min}} \quad (10)$$

Terms W_1 , W_2 , W_3 , W_4 , and W_5 represent the weights correspond to BP, BTE, CO, UHC, and NOx, respectively. $BP_{\min}$, $BTE_{\min}$, $CO_{\min}$, $UHC_{\min}$ and $NOx_{\min}$ are the minimal values, while $BP_{\max}$, $BTE_{\max}$, $CO_{\max}$, $UHC_{\max}$ and $NOx_{\max}$ are extracted from the individual objective functions of BP, BTE, CO, UHC, and NOx, respectively. DFA_{BP} , DFA_{BTE} , DFA_{CO} , DFA_{UHC} and DFA_{NOx} represent the desirability function values of BP, BTE, UHC, CO and NOx, respectively. In Eq. (5), terms such as BP, BTE, CO, UHC, and NOx refer to Eqs. (3a), (3b) and (4a), 4b and 4c. The weights for individual objective functions are determined based on six case studies. Case 1 assigns equal importance to all outputs, while Case 2–6 assign maximum importance to one output, with a weight of 0.6, while keeping the rest at a minimal value of 0.1. The best set of parameters is identified through these instances corresponding to the computed highest composite DFA value ($DFA_{\text{Composite}}$). The Rao-3 algorithm and DFA techniques are applied to determine the optimal condition by solving Eq. (5). Table 13 presents the findings of the most suitable parameters for engine testing and environmental friendliness, emphasizing improved performance (BP and BTE) and emission characteristics (UHC, CO, and NOx).

The fitness values or desirability function value (composite: considering all responses or $DFA_{\text{Composite}}$) for the maximization of corresponding Eq. (5) are determined for each case study (Case 1 to 6). It was noted that the maximum fitness value was considered as an optimized condition for all outputs. The fitness value corresponding to the six case studies were examined. Assigning equal weights for all outputs representing Case 1 resulted in a fitness value of 0.9292, 0.9439 for assigning maximum importance to BP representing Case 2, 0.9373 for assigning maximum importance that maximizes the BTE representing case 3, 0.9317 for assigning maximum weight fraction that minimizes the CO representing Case 4, 0.9556 for assigning maximum weight fraction that minimizes UHC representing Case 5, and 0.9483 for assigning maximum weight fraction that minimizes the NOx emissions representing Case 6, respectively (refer to Table 13).

The fitness values were evaluated for all the case studies (Case 1 to Case 6) and the resulting maximum fitness value corresponding to Case 5 (Maximum weight for UHC) is treated as the optimal condition (refer to Table 13). The recommended optimal parametric conditions (21.34 vol% of blend fuel, 63.43 ppm of nanoparticle, 1435.18 rpm of engine speed and 24.35 % for engine load) were subjected to practical experiments. Experiments corresponding to Case 5 (21.34 vol% of blend fuel, 64 ppm of nanoparticle, 1435 rpm of engine speed and 24 % for engine load) resulted in BP, BTE, CO, UHC, and NOx values of 8.2 kW, 29.4 %, 66.2 ppm, 2.82 ppm, and 701.4 ppm, respectively. The deviation in Rao algorithm predictions from experimental values resulted in an absolute percent error of 4.63 % for BP, 3.98 % for BTE, 2.46 % for CO, 5.32 % for UHC, and 0.85 % for NOx emissions, respectively. However, RSM based DFA

Table 13
Summary of optimized conditions for diesel engine and emission characteristics.

Case study	Method	Input variable				Output variable					Fitness value
		A: Blend type (Vol. %)	B: Nanoparticle (ppm)	C: Engine speed (rpm)	D: Load (%)	BP (KW)	BTE (%)	CO (ppm)	UHC (ppm)	NOx	
Case 1: Equal weight for all output (1/5 = 0.2)	Rao-3	18.81	66.76	1366.75	27.77	8.48	29.17	65.3	2.71	687.1	0.9292
	DFA	21.79	70.96	1362.46	23.64	7.20	26.47	62.80	2.70	669.78	0.9229
Case 2: Maximum weight for BP = 0.6 and rest (0.1 each)	Rao-3	17.7	74.28	1547.49	29.89	10.34	31.95	69.97	2.86	694.80	0.9439
	DFA	21.53	73.17	1406.54	30.00	9.43	30.12	67.72	2.76	675.01	0.9382
Case 3: Maximum weight for BTE = 0.6 and rest (0.1 each)	Rao-3	16.34	54.15	1547.39	29.58	10.27	33.54	71.46	2.77	749.97	0.9373
	DFA	17.50	57.21	1487.43	28.72	9.58	31.94	68.93	2.73	730.23	0.9351
Case 4: Maximum weight for CO = 0.6 and rest (0.1 each)	Rao-3	12.68	64.17	1403.67	19.29	6.05	24.45	58.22	2.80	681.75	0.9317
	DFA	21.83	68.92	1352.35	14.74	4.43	19.15	58.62	2.67	671.68	0.9158
Case 5: Maximum weight for UHC = 0.6 and rest (0.1 each)	Rao-3	21.34	63.43	1435.18	24.35	7.82	28.23	64.57	2.67	707.38	0.9556
	DFA	21.40	61.35	1378.71	21.51	6.64	25.81	62.15	2.65	705.19	0.9553
Case 6: Maximum weight for NOX = 0.6 and rest (0.1 each)	Rao-3	24.91	79.4	1338.9	25.29	7.60	26.79	64.17	2.79	630.86	0.9483
	DFA	26.55	80.00	1339.04	20.72	6.23	23.69	62.67	2.80	616.21	0.9449

determined optimal conditions examined experimentally resulted in BP of 7.3 kW, BTE of 25.96 %, CO of 64.5 ppm, UHC of 2.64 ppm, and NOx of 705.4 ppm corresponding to a fuel blend of 21.34 % vol., ZnO additive of 61.35 ppm, engine load of 21.5 %, and engine speed of 1380 rpm corresponding to Case 5 determined the highest desirability function value of 0.9553 (refer to Table 13). The optimal values of all outputs fell within less than 6 %, indicating that the Rao algorithm is efficient for performing optimization tasks.

4. Conclusion

This study investigated the performance and emission optimization of a compression ignition (CI) engine using ZnO nanoparticle-enriched castor-neem biodiesel blends. A hybrid modelling approach combining RSM with the Rao-3 optimization algorithm was employed, proving to be reliable and effective in refining the engine’s operational parameters.

The experimental design using RSM efficiently determined the impact of key factors such as biodiesel blend ratio, nanoparticle concentration, engine load, and speed on performance metrics like BP, BTE, and emissions (CO, UHC, and NOx). All five models developed for performance and emission characteristics produced better R² value (close to 1), depicting that the models are statistically adequate. The experimental and model predicted data points were close to the ideal trend line depicting the models statistical adequacy that could predict with minimal deviation. Optimal conditions identified by RSM resulted in a brake power of 7.3 kW, brake thermal efficiency of 25.96 %, CO emissions of 64.5 ppm, UHC emissions of 2.64 ppm, and NOx emissions of 705.4 ppm, with a desirability index of 0.9553.

Further refinement using the Rao-3 algorithm identified globally optimal operating conditions: fuel blend ratio of 21.34 vol%, ZnO nanoparticle dosage of 63.43 ppm, engine speed of 1435.18 rpm, and load of 24.35 %. These settings improved the desirability index to 0.9556. Experimental validation under these optimized conditions resulted in a brake power of 8.2 kW, brake thermal efficiency of 29.4 %, CO emissions of 66.2 ppm, UHC emissions of 2.82 ppm, and NOx emissions of 701.4 ppm. The close agreement between predicted and measured values, with the Rao-3 model showing lower absolute percentage errors compared to RSM predictions, confirmed the robustness and reliability of the optimization framework. The study shows that adding ZnO nanoparticles to castor-neem biodiesel blends improves combustion efficiency, engine performance, and reduces emissions. The integration of RSM and Rao-3 algorithms is effective for optimizing internal combustion engine systems, leading to more energy-efficient and environmentally friendly technologies.

Future studies should focus on the long-term durability and wear characteristics of engines using nanoparticle-enriched biofuels, especially under real-world driving conditions. Investigating the combined effects of multi-metal oxide nanoparticles like CeO₂, Al₂O₃, and TiO₂ could offer valuable insights into improving combustion efficiency and reducing emissions. Furthermore, exploring advanced combustion strategies such as exhaust gas recirculation (EGR) and varying injection pressures may uncover new approaches to mitigate emissions. Conducting lifecycle assessments (LCA) and techno-economic analyses (TEA) of nanoparticle-enhanced biodiesel blends would be essential to validate their feasibility and environmental benefits for widespread adoption in the transportation and energy sectors.

CRediT authorship contribution statement

Chao-zhe Zhu: Writing – review & editing, Visualization. **Olusegun D. Samuel:** Writing – original draft, Methodology, Investigation, Formal analysis, Conceptualization. **Manjunath Patel G C:** Writing – review & editing, Validation, Formal analysis. **Oguzhan Der:** Writing – review & editing. **Mohamed Abbas:** Writing – review & editing, Visualization. **Fayaz Hussain:** Writing – review & editing, Visualization. **Tin Tin Ting:** Writing – review & editing, Visualization.

Declaration of competing interest

The authors declare there is no potential conflict of interest.

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Nomenclature

Symbol/Abbreviation	Description
BP	Brake Power (kW)
BTE	Brake Thermal Efficiency (%)
CO	Carbon Monoxide Emission (ppm)
UHC	Unburnt Hydrocarbon Emission (ppm)
NOx	Oxides of Nitrogen Emission (ppm)

(continued on next page)

(continued)

Symbol/Abbreviation	Description
CNSOME	Castor-Neem Seed Oil Methyl Ester
ZnO	Zinc Oxide Nanoparticles
RSM	Response Surface Methodology
Rao-3	Third Variant of Rao Optimization Algorithm
DoE	Design of Experiment
CCRD	Central Composite Rotatable Design
DFA	Desirability Function Approach
PI	Performance Indices
EAs	Emission Attributes
LCN	Low-Carbon Nanoparticle-Doped Fuel

Appendix 1. Fatty acid composition of CNSOME and transesterification condition

Appendix A1. Fatty acid composition of CNSOME

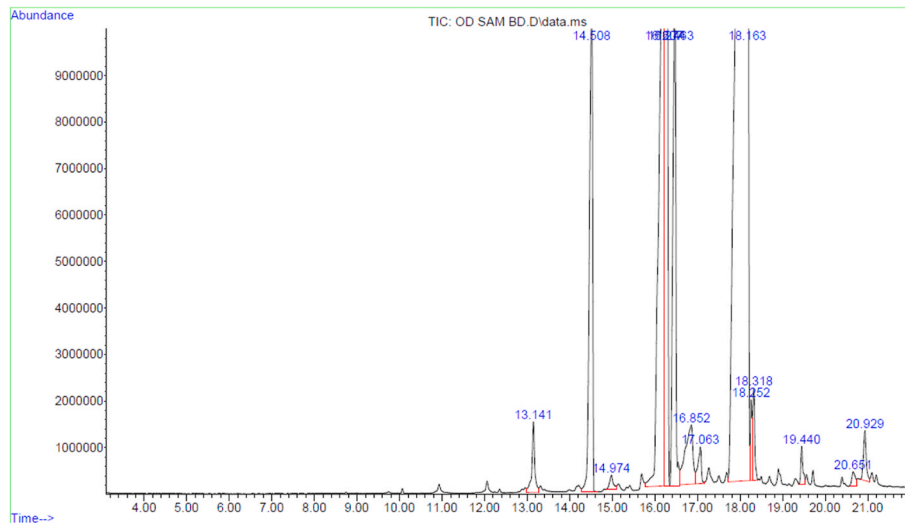


Fig. A1. FAME analysis/GCMS Analysis of CNSOME/Biodiesel.

Appendix A2. transesterification condition

Table A1

Process conditions for the transesterification

Transesterification variables (TVs)						Optimum conditions			
Reaction	Castor/neem seed oil ratio (CNSO)	HC (wt.%)	RT(h)	MR	RET (°C)	HC	RT (h)	MR	RET (°C)
Transesterification	20 % neem seed oil +80 castor seed oil (N20)	12–20	1.0–3.0	4–10	50–70	14.3	1.58	10	59.4

HC = heterogeneous catalyst; RT = reaction time; MR = molar ratio, RET = retention time.

Appendix 3. Standard deviation and uncertainty

Tables A2 and A3 show the standard deviation (SD) of key measurable values and the uncertainty values (UVs). The SD and UVs were estimated using Eqs. (A1) and (A2), respectively.

$$SD = \sqrt{\frac{\sum (X_L - \text{Mean})^2}{n - 1}} \quad (\text{A1})$$

$$UVs = \frac{2\sigma}{\text{Mean}} * 100 \quad (\text{A2})$$

where X_L , n , and σ are the measured value, total number of observation, and standard deviation, respectively

Table A2
Standard deviation of key measured values

	Load	Speed (N)	Mf	LHV
Σ	$= \sqrt{\frac{2000}{29}}$ = 8.3045	$= \sqrt{\frac{2160000}{29}}$ = 272.9153	$= \sqrt{\frac{0.00003192214}{29}}$ = 0.001049	$= \sqrt{\frac{18.599}{29}}$ = 0.80084

Appendix 4. Uncertainty for BP and BTE

The uncertainties for BP and BTE were estimated using Eqs. (A3) and (A4)

$$\text{Uncertainty for Brake Power, BP} = \sqrt{\left(\frac{\Delta N}{N}\right)^2 + \left(\frac{\Delta L}{L}\right)^2} \quad \text{A3}$$

$$\text{Uncertainty for Brake thermal efficiency (BTE)} = \sqrt{(\Delta \text{BP})^2 + (\Delta \text{MF})^2 + (\Delta \text{LHV})^2} \quad \text{A4}$$

Table A3
Uncertainty of key measured values

	Load	Speed	M _f	LHV
In (%)	$\frac{2 \times 8.3045 \times 100}{20}$ = 83.05 0.8305	$\frac{2 \times 272.9153 \times 100}{1400}$ = 38.99 0.3899	$\frac{2 \times 0.001049 \times 100}{0.003977}$ = 52.75 0.5275	$\frac{2 \times 0.80084 \times 100}{39.27}$ = 4.079 0.04079

Appendix 4. Uncertainty of exhaust emission

The uncertainty of key exhaust emission (EE) was estimated using Eq. (A5) as reported elsewhere [39,81]. Table A4 presents the uncertainty of EE.

$$\text{Uncertainty (\%)} = \left(\frac{\text{Instrument uncertainty}}{\text{Mean}} \right) * 100 \quad (\text{A5})$$

Table A4
Uncertainty of emission features

Emission	Instrument uncertainty (ppm) (±)	Mean (ppm)	Uncertainty (%)
CO	2	59.13	3.38
UHC	0.05	3.04	1.64
NO _x	5	750.80	0.67

Data availability

Data will be made available on request.

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