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Cerium Oxide Blended Biodiesel: Machine Learning and Response Surface Methodology for Prediction of Responses

Padmakar Kabudake[1*], Yashwant Kharade[2], Rakhamaji Gavahane[3] and Milind Mhaske[1]

[1]*Mechanical Engineering Department, Pravara Rural Engineering College, Loni, Ahmednagar, 413736, India*
[2]*Mechanical Engineering Department, Shri Chhatrapati Shivaji Maharaj College of Engineering, Nepti, Ahmednagar, 414005, India.*
[3]*Mechanical Engineering Department, Amrutvahini College of Engineering, Sangamner, Ahmednagar, 422608, India.*

Abstract

Because of the rising demand for diesel, researchers are looking into finding a new alternative fuel. Biodiesel is an excellent alternative to neat diesel due to its renewable, biodegradable, and non-toxic nature. However, its response characteristics, such as brake thermal efficiency (BTE) and brake-specific fuel consumption (BSFC) should be predicted correctly. Thus, the present work includes the production of biodiesel from cottonseed oil with two-step transesterification and the investigation of response characteristics for a single-cylinder diesel engine fueled with Cerium oxide, i.e. nanoparticle additive (NA), which is blended cottonseed oil biodiesel. Compression ratio (CR) and NA levels have varied from 16 to 18 and 50 to 100 ppm, respectively. Input parameters, namely CR and NA levels are considered for the present investigation. The present study presents a novel method that uses deep learning-based surrogate modelling, a machine learning (ML) technique to forecast the responses. The optimum operating conditions are a CR of 18 and an NA level of 83.877 ppm. The study results demonstrate that the deep learning model provides a convincing substitute for classical regression models such as Random Forest, Decision Tree, Support Vector Machines, Gradient Boosting, and K-Nearest Neighbor Regressor. Further, multi-objective optimization of input parameters is performed using the desirability function approach. The optimized parameters were attained at a composite desirability of 0.847. Lastly, confirmation experiments are performed to validate the results of non-linear regression models and found satisfactory with an error percentage of less than five.

Keywords: Cottonseed oil, Nanoparticle additive, Brake Thermal Efficiency, Brake Specific Fuel Consumption, Deep Learning, Surrogate modelling

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Contact
* Corresponding author
Padmakar Kabudke
kabudkepadmakar@gmail.com
Address: Pravara Rural Engineering College, Loni, Ahmednagar, 413736, India.

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1. Introduction

Everyday operations require fossil fuels as an energy source for running compression ignition (CI) engines (1). These CI engines guarantee power production in agriculture, irrigation, and transportation fields. As a result, in today's globe, fossil fuels such as crude oil, natural gas, and coal are in great demand; nevertheless, their reserves are decreasing. As a result, the exhaustion of diesel fuel and the imposition of tight pollution laws are significant concerns for society. Therefore, there is a need to develop other energy sources that will last a long time (2). In recent times, biodiesel appears to be an excellent replacement for established fuels (3). Biodiesel is a non-toxic, renewable, and biodegradable fuel that offers a cost-effective alternative to conventional fuels (4). Also, because the feedstocks for biodiesel synthesis are edible, non-edible vegetable oil and animal fats, biodiesel may be utilized as a fuel in CI engines as an alternative to diesel to support rural development and economics. However, some concerns need to be addressed before the actual utilization of biodiesel as a fuel. These are: (i) Biodiesel should not be utilized directly due to its increased viscosity, (ii) Also, after burning of biodiesel fewer contaminants are emitted, which are less harmful to human health (5). Nevertheless, the use of biodiesel has improved lubricity, which benefits engine rotating components. However, biodiesel's performance and combustion characteristics should be further evaluated. As a result, this paper aims to improve its fuel characteristics as closely as possible to those of neat diesel-fueled engines.

Various researchers have studied the characteristics of CI engines when fueled with biofuels (6). Arumugam et al. investigated the substitution of artificial lubricant with rapeseed oil-based bio-lubricants in an engine (7). They found that a combination of biofuel/bio-lubricant reduced wear and ash content compared to a traditional fuel-lubricant combination. Selvan et al. performed an experimental investigation to conduct combustion, performance, and emission analysis of Cerium Oxide Nanoparticles and Carbon Nanotubes nanoparticle additives in di-esterol blends (8). They found that adding additives increased cylinder gas pressure compared to neat di-esterol blends. Bridjesh et al. studied the performance properties of variable compression ratio (VCR) diesel engines using a Calophyllum inophyllum biodiesel blend (9). The result showed minimized brake thermal efficiency (BTE) and increased brake-specific fuel consumption (BSFC) using neat diesel. Suresh et al. comprehensively evaluated biodiesel production from several non-edible oils in terms of combustion, performance, and emission characteristics of VCR diesel engines (10). As per their investigation, better brake fuel efficiency and minimization in fuel utilization are possible with blended biodiesels. Murugapoopathi and Vasudevan performed energy and exergy analysis of biodiesel-fueled engines at several fuel blends and compression ratios (CRs) combinations (11). They found optimum engine settings based on the input factors. They also found that a combination of CR20, B20,
and B40 performs better at 80% load for esters of seed oil in a mixture with diesel. Khatri et al. experimented to study the influence of zinc oxide (ZnO) nanoparticles in addition to diesel on the properties of diesel engines (12). They found a 15.58% increase in BTE and an 11.11% increase in BSFC with additives. Also, they found that the emissions are significantly reduced. Hussain et al. studied a diesel engine's performance properties using a soybean-diesel mixture with cerium-coated zinc oxide nanoparticles (13). At the 50 ppm additive level, the BTE increased by 26.66% and BSFC reduced by 21.81%. Subramani and Karuppusamy conducted experiments to check VCR diesel engine characteristics using biofuel (B20) blended with nano-additives (14). They found that BTE increased by 3.62%, and BSFC decreased by 3.3% more than neat diesel. Also, there is a reduction in NOx emissions. Rajak et al. blended base fuel with oil to study the feasibility of the product as a fuel substitute in CI engines (15). They found that a maximum BTE of 34.4% and the lowest BSFS of 738.29g/kWh is attainable with the use of the blended fuels. Vali et al. optimized engine parameters to improve the performance, emission, and combustion characteristics of diesel engines using a central composite rotating design (16). The optimum output responses are BTE of 30.75% and brake-specific energy consumption of 13.92 MJ/kW.hr.

The review paper by Shelare et al. discusses waste biodiesel production, nano-additives, and the applications of Internet-of-things (IoT), artificial intelligence (AI), and machine learning (ML) in biofuels. These advancements can promote biodiesel as a cleaner, renewable energy source (17). Further, fast and precise modelling tools are needed for design, optimization, monitoring, and control in the production and use of biodiesel. Artificial neural network (ANN) technology, in particular, has demonstrated improved predictive potential in data-driven ML techniques. ANN is frequently utilized in biodiesel research to solve optimization, control, monitoring, and function approximation issues. In addition to reviewing several ML technology applications with an emphasis on ANN, the researchers also discussed the benefits and drawbacks of applying ML to biodiesel research. Future research should concentrate on real-time process control and monitoring to improve environmental sustainability, economic viability, and production efficiency (18). In automotive applications, ANNs are a common predictive tool, especially for intricate and expensive systems (19).

Li et al. developed a response surface optimization model for diesel-biodiesel hybrid engines. They reduced emissions while maximizing engine performance (20). Dharmalingam et al. utilized a Bayesian neural network and response surface methodology to predict diesel engine performance with waste cooking oil biodiesel, showcasing improved accuracy over traditional methods (21). Response surface methodology aids in predicting the performance of diesel engines with biodiesel-nanoparticle blends. Machine learning can enhance prediction accuracy for cerium oxide blended biodiesel in compression ignition engines (22). ML algorithms like random forest and AdaBoost are effective for predicting biodiesel production responses, as demonstrated by Gupta et al. (23). Increased performance and decreased emissions in blended biodiesel with EGR were observed by Selvam et al. (24). They found that novel nano-additives improved engine characteristics and reduced emissions significantly. Murugapoopathi et al. carried out prediction and evaluation of performance and emission analysis using biodiesel blends. Comparison with standard diesel using a response surface methodology approach was also performed in their research (25).

Doğan et al. examined the impact of adding nanoparticles to diesel and heavy fuel oil blends on engine performance, with a focus on enhancing efficiency and reducing environmental harm. Detailed experiments demonstrated the effects of nanoparticles on engine power, fuel consumption, exhaust gas temperature, engine temperature, and pollutant emissions, aiming to comprehend the potential for more sustainable fuel use. Comparing various fuel blends with nanoparticles revealed a decrease in energy loss and an improvement in engine efficiency, signaling progress towards mitigating the negative environmental effects of fuel consumption (6). Koçyiğit et al. investigated the impact of adding ethanol and propolis to diesel fuel on engine performance and emissions under various load conditions. They suggested using propolis as a novel bio-based additive to reduce environmental pollution in diesel fuel. The analysis examined how propolis and ethanol inclusion affected engine parameters and emissions, providing insights into sustainable fuel options. They also showcased propolis's antioxidant properties and its benefits as an additive in diesel fuel (26). Özel et al. discussed the impact of ceramic coatings on diesel engine emissions like CO, CO_2, HC, and NO_x using TBC methods with Cr_2O_3 and Al_2O_3 powders. Taguchi analysis is applied to optimize the influence of coatings on emissions, improving engine performance and environmental compliance. They introduced Taguchi optimization and ANOVA tests to analyze the effects of ceramic coatings on emissions, identifying factors that affect exhaust values (27). They further examined the impact of thermal barrier coatings on diesel engine performance using the Taguchi method for optimization. They presented a new approach to quality processes in engineering by applying Taguchi's loss function to thermal barrier coatings. They also determined optimal values for engine torque, power, and fuel consumption by testing different coating materials and engine speeds (28). Vural et al. examined the effects of blending hexane and water with diesel fuel on emissions and performance in ceramic-coated and uncoated diesel engines using the Taguchi optimization method. The research revealed that adding hexane and water to diesel fuel can enhance emission and performance parameters, particularly in ceramic-coated engines at a 4 kW brake load. Although blending hexane and water with diesel fuel generally improved emission and performance parameters, pure diesel fuel remained superior for brake thermal efficiency. ANOVA testing identified brake load, fuel type, and engine coating as significant factors affecting emissions and performance, offering a statistical foundation for optimizing diesel engine operation with hexane-water-diesel blends (29).

From the reviewed literature, it is concluded that the engine performance can be controlled simultaneously by tuning CR and NA levels in biodiesel. Also, more focus should be given to improvement in thermal efficiency and minimization in fuel utilization of CI engines. However, limited studies have been reported on optimizing engine variables for improvement in BTE and BSFC. To the best of the researcher's knowledge, no studies have been reported on the use of ML techniques in the prediction of response characteristics. Thus, the objectives of the present study are to perform a critical analysis of the effects of CR and the level of NA on the response characteristics of biodiesel-fueled CI engines. Deep-learning-based surrogate modelling, i.e. ML techniques and Response surface methodology (RSM) are used for the generation of non-linear models of response characteristics. The methodology of the present work is discussed in the next section.

2. Methodology

The biodiesel mixed with NA was prepared for performing experiments in a VCR diesel engine. The methodology of the present work is shown in Figure 1.

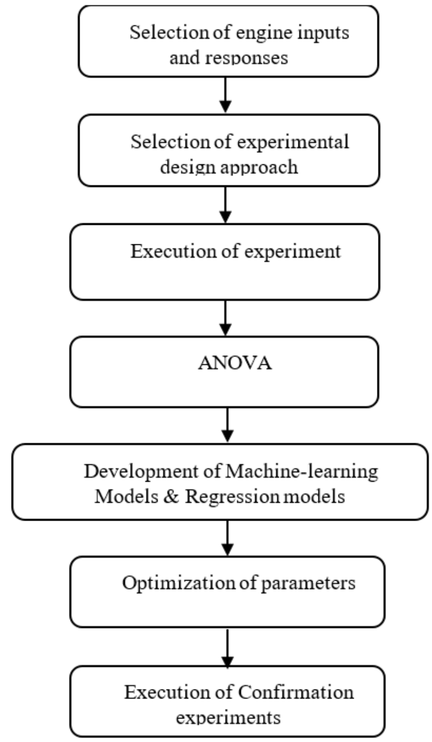


Fig. 1. Methodology of the present work

2.1. Materials

The liquefied fuel used in the experiments comprised cottonseed oil and neat diesel. Apex Innovation Pvt. Ltd. India offered 99.5 per cent pure Analytic Quality Methanol Merck and Potassium Hydroxide (KOH). In Table 1, the fatty acid profile of cottonseeds was listed, which was analyzed at Nikhil Analysis and Research Pvt. Ltd., Sangli, India. Table 1 lists the fatty acid composition of cottonseed oil fatty acid.

Table 1. Cottonseed oil fatty acid composition.

Fatty Acidulous name	Construction	Weight %
Myristic Acidulous	C14:0	00.53
Palmitic Acidulous	C16:0	10.33
Stearic Acidulous	C18:0	03.64
Oleic Acidulous	C18:1	32.82
Linoleic Acidulous	C18:2	39.29

2.1.1. Preparation of Biodiesel

The biodiesel preparation starts from transesterification to drying of ester. During the transesterification reaction, methanol reacts with KOH to form ester and glycerol. The prepared biodiesel was blended with a nanoparticle additive in the present investigation. Methanol/oil molar ratio (4:1-8:1), catalyst concentration (0.5-2 per cent), temperature (50-70°C), and catalyst KOH were the reaction variables employed. In a batch reactor, the efficiency of transesterification increased with increasing temperature up to 60°C. Ultrasonication was used to prepare nanoparticle cerium oxide concentration with a biodiesel blend. NAs were dispersed into the water in biofuel, resulting in 50 ppm, 75 ppm, and 100 ppm blends of biofuels. The preparation process of biofuel with NA is shown in Figure 2. Properties of biofuels were tabulated in Table 2.

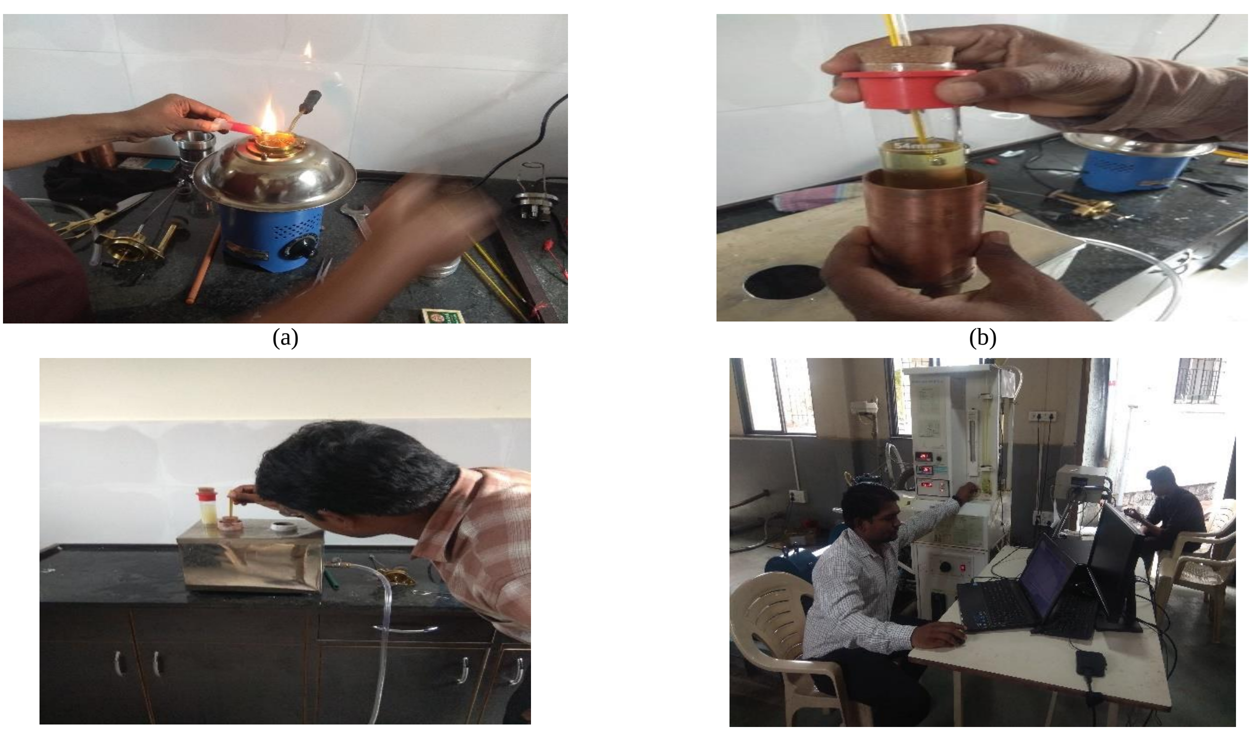
Uncertainty analysis was performed to establish the confidence level of acquired results. The uncertainty ratio was dependent on equipment selection and test arrangement. Uncertainty in measured parameters was tabulated in Table 3.

2.2.2 Experimental Setup

A water-cooled individual-cylinder VCR engine connected dynamometer with all essential equipment, including the Kirloskar computer interface diesel engine, was set up. Then, the CR of the engine was tuned with the auxiliary piston using a screw rod and hand wheel assembly. A marked scale was provided to the screw rod for varying CRs. The experiments were performed on individual cylinder engines with CR16, CR17, and CR18 producing 3.5 kW power (1500 rpm). Then, the performance analysis was carried out using the diesel blends at the additive levels of 50, 75, and 100 ppm. Figure 3 shows the experimental setup and schematic diagram of the test rig. Table 4 listed the detailed specifications of the VCR diesel engine, and the properties of fuel used were tabulated in Table 4. Engine Soft LV collects, stores, and analyses data during tests using numerous measurement sensors utilizing engine performance analysis software with automated data editing tools. For this experiment, a strain gauge-type load cell, an eddy current-type dynamometer, and a loading unit were used to measure the load. The fuel flow rate was determined by utilizing a load cell to calculate the fuel weight loss in the fuel tank. It was ensured that there was sufficient water flow before starting the engine.

Table 2. Properties of fuel

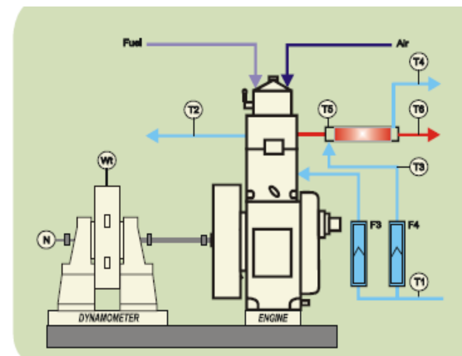
Fuel properties	Standard	Diesel	CB100	CB20	CB20+50ppm	CB20+100ppm
Density @25 0C (gm/cm3)	ASTM D287	0.83	0.874	0.8388	0.848	0.852
Specific Gravity	ASTM D287	0.83	0.874	0.8388	0.848	0.852
Gross Calorific Value Cal/gm	ASTM D 4809	44000	39045	43009	43350	43380
Flash Point 0C	ASTM D 93-58T	66	130	91	94	96
Cetane number	ASTM D 93-58T	49	56	52	52	51.5
Cloud Point 0C	ASTM-D 97	-6	0	-4.8	-4.2	-3.6
Pour Point 0C	ASTM-D 97	-10	-4	-8.8	-8.2	-7.6
Kinematic Viscosity @40 0C cst	ASTM D 445	2.95	4.31	3.53	5.64	5.68
FFA %	> 2.5	-	0.53	-	-	0



(a) (b) (c) (d)

Fig. 2. Measurements (a) Fire Point, (b) Cloud Point Measurement, (c) Flash Point Measurement, and (d) Experimentation on single-cylinder VCR Diesel engine

(a)



(b)

Fig. 3. Test rig

Table 3. Uncertainty in measured parameters

Parameters	Accuracies	Uncertainty
Air flow rate	±1.0 cm3/h	± 0.15%
Fuel consumption	±2.0 g/h	± 0.10%
Engine speed	± 10 rpm	± 0.5%
Load	± 0.15 N	± 0.15%
Power	-	± 0.15%
Temperatures	± 1 ^{0} C	± 0.10%

Table 4. Specification of engine

No. of cylinder	One
No. of stroke	Four
Fuel type	Diesel
Power of engine	3.5 kW@1500 rpm
Type	Constant speed
Stroke length	111 mm
Bore diameter	87.5 mm
Connecting rod length	234 mm
Cooling Method	Water Cooled
Compression ratio	16
Swept volume	661.45 cm^3

2.2.3 Response Surface Methodology

RSM is a statistical experimental design technique for modelling and optimizing real-world problems. The present study examined CR and NA levels as input parameters. These parameters could affect response characteristics such as BTE and BSFC. Thus, quadratic regression models of response characteristics were developed using the central composite design (CCD) matrix technique of RSM. Experimental design was performed with the help of Design-Expert V13.0 software. This software offers an effective solution for designing processes and predicting their behavioural characteristics under different conditions. In the present study, two parameters are varied at three levels, resulting in a matrix as tabulated in Table 5, which lists input parameters and average values of response characteristics at a load level of 100%.

In addition to the evaluation metrics discussed, it is pertinent to provide insight into the coefficient of determination (R^2) values obtained during model validation. The R^2 serves as a measure of how well the model fits the observed data. In our study, the R^2 values for BTE and BSFC are 0.9938 and 0.9973. These values provide further validation of the model's predictive capability and its suitability for the analysis of responses.

Table 5. Test parameters

Case No.	Input Parameter		Response Characteristics	
	Compression ratio	NA level	BTE (%)	BSFC (kg/kWh)
1	17	100	26.77	0.31
2	16	75	26.11	0.3
3	16	50	26.23	0.33
4	18	75	27.4	0.27
5	17	50	26.48	0.32
6	16	100	26.77	0.31
7	18	50	28.06	0.29
8	18	100	28.1	0.29
9	17	75	26.16	0.291

After conducting experiments according to CCD, analysis of variance (ANOVA) was used to clarify statistical parameters, namely, R^2, Adjusted R^2, Predicted R^2, F-value, and p-value. Significant parameters were represented by parameters having a p-value less than 0.05.

2.2.4 Machine Learning Technique

2.2.4.1 Architecture

The neural network architecture used for surrogate modelling in this study is a key element within the deep learning framework. The primary objective of this design was to effectively capture the intricate and non-linear connections that exist for the response characteristics of biofuels. The architectural design often used is a deep feed forward neural network, which is sometimes referred to as a multi-layer perceptron (MLP). The architecture consists of nine concealed layers, each containing a variable number of neurons or nodes, facilitating the representation of complex patterns and relationships present in the data as shown in Figure 4. MLP has four major components- the fully connected layer, dropout layer, skip connections and outer layer. The input layer is a combination of normalized vectors of input parameters. Advanced activation functions, such as Rectified Linear Units (ReLU) are used to improve the performance of models. The output layer is designed to cater to particular goals, generally offering forecasts for BTE and BSFC. Regularization methods, such as dropout and batch normalization, are used to mitigate the issue of over fitting. Skip connection is added for smooth learning and to control vanishing and exploding gradients. The determination of the architecture's complexity, the number of layers, and the hyper parameters is conducted via a process of testing and optimization. This is done to attain a surrogate model for the analysis that is both highly accurate and efficient. The flexibility and generalization capabilities of the neural network design provide it a potent instrument for correctly representing the response characteristics of biofuel.

Thus, in the present architecture, the total number of trainable parameters became 23,945 from 7500 training data points. Model over fitting is handled using dropout and cross-validation-based early stopping.

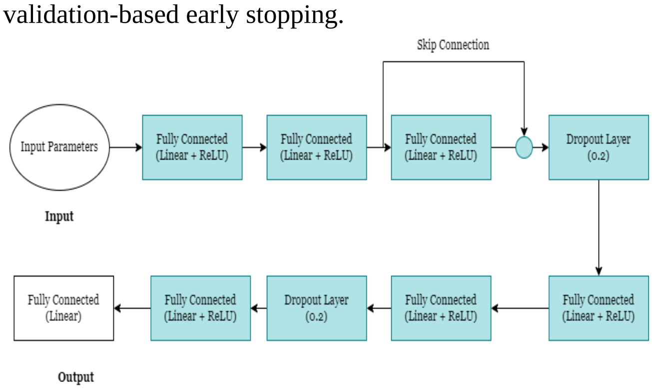


Fig. 4 Deep Neural Network Framework

2.2.4.2 Training and Validation

Design space investigation is a method to recognize the effect of the input variables on responses and analyze the complicated association between them. Thus, the training phase of the deep learning model is a crucial component in this study, during which the neural network acquires the ability to approximate the intricate connections between input parameters namely Nt, Nn, Na, and Nh and the response namely, BTE and BSFC. Initially, a complete dataset containing 10211 data points was randomly split into training data (7500) and test data (2711). The training procedure begins with the use of a meticulously pre-processed dataset, whereby the inputs include a range of variables, compression ratio, and NA level. The model repeatedly analyzed the given data by doing forward and backward runs. During this process, the model adjusts its internal weights and biases to reduce the discrepancy between its predictions and the actual findings. The process of training involves many epochs or iterations when the model is repeatedly exposed to the data to enhance its predicting skills. The optimization of hyper parameters, such as learning rates and batch sizes, was performed to achieve effective convergence and enhance the generalization capabilities of the model. The result was a deep learning model that can make exact predictions about the performance of pressure vessels. This capability was acquired via the model's acquisition of information from the training data. Consequently, the model facilitates the efficient and accurate analysis, design, and optimization of pressure vessel systems.

To enhance prediction accuracy, a group of deep learning networks were trained, since they were seen to be more precise than individual predictors, due to the lack of extensive data. To achieve this objective, 5-fold cross-validation was used and a separate deep neural network on each dataset fold. Each fold dataset was thereafter partitioned into a training dataset (90%) and a validation dataset (10%). The multiple trained networks' predictions were averaged to produce the final values of the BTE and BSFC for a specific parameter set. Through the process of conducting experiments with various loss functions and learning rates, it was determined that the Lasso (L1) loss function outperformed other alternatives when paired with a learning rate of 0.001. The model was trained using the Adam optimizer with Xavier/He initialization. Figure 5 shows an ensemble of learning models.

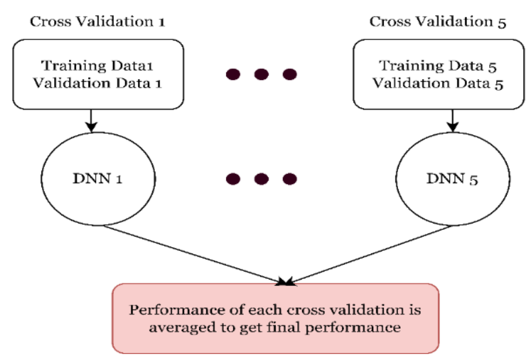


Fig. 5 Ensemble of learning models

2.2.4.3 Model Evaluation

The assessment of the deep learning-based surrogate model's effectiveness in pressure vessel examination necessitates the use of distinct measures to measure its precision and dependability. Metrics play a crucial role in quantifying the accuracy of a model's predictions about pressure vessel behaviour. In the present investigation, MAE and RMSE were used for model evaluation, which is computed as per Eq. (1) and Eq. (2) respectively.

$$MAE = \frac{1}{n} \times \sum \left(\left|(\sigma_{actual} - \sigma_{predicted})\right|\right) \tag{1}$$

$$RMSE = \sqrt{\frac{1}{n} \times \sum \left(\frac{(\sigma_{actual} - \sigma_{predicted})^2}{1}\right)} \tag{2}$$

Where:

n represents the total number of data points inside the dataset. *Σ denotes* the summation of all data points.

σ_{actual} = actual value

$\sigma_{predicted}$ = predicted value

The expression $(\sigma_{actual} - \sigma_{predicted})^2$ is used to compute the squared discrepancy between the observed (σ_{actual}) value and the expected ($\sigma_{predicted}$) value for each data point.

It provided valuable information on the quality of the model and its capacity to accurately represent the differences in stress distributions and deformations. The RMSE had the favorable attribute of being easily interpretable due to its correspondence with the units of the target variable. The RMSE exhibited scale independence, making it appropriate for the comparative assessment of model correctness across diverse datasets and target variables. The magnitude of mistakes was more effectively penalized by the RMSE in comparison to the MAE due to the squaring of errors. The RMSE was a number that was always non-negative or zero. A score of zero indicated that the model's predictions align perfectly with the actual data. The RMSE was susceptible to the influence of outliers due to the squaring of mistakes, which amplifies the impact of larger errors in the overall computation. The RMSE was often used to assess the efficacy of regression models and to ascertain the superior predictive capabilities of various models.

Accuracy was calculated as a percentage of the number of samples whose MAE was within an acceptable error of 10%. For comparison purposes, the Random Forest and Gradient Boosting Regressors models were developed using the same training dataset.

3. Results and Discussion

This section focuses on the impact of diesel engine input variables on two response characteristics.

3.1 Engine Performance Test

3.1.1 Brake thermal efficiency

BTE measures the performance of the engine. The primary purpose of this study is to test the efficiency of cottonseed biofuel with NA. The influence of the percentage of biofuel mixture on performance was observed for various loads. In all running situations with changing loads, the BTE of biofuel is between 2 to 30 per cent, as shown in Figure 6. The plotted curve in Figure 6 shows that efficiency increases with an increase in load from 19.6 Nm to 117.6 Nm.

ANOVA values for BTE analysis are tabulated in Table 6. Also, the regression model for BTE is given in Eq. (3). It is found that both input parameters significantly affect BTE. From the surface plot shown in Figure 7, it is observed that BTE increases with an increase in CR and NA levels. A similar trend is observed for variation in CR is given in the published literature using different biofuel and NA combinations (14–16,30–33). Higher efficiency with increased NA level is attributed to the high surface area of NA, their catalytic effect, more excellent fuel-oxidizer contact, and higher rate of reaction.

3.1.2 Brake Specific Fuel Consumption

In all running situations with changing loads, the BSFC of biofuel is between 0.2 to 1 kg/kWh. During experimentation value occurs at higher side because of zero brake power (No load condition). The plotted curve in Figure 6 shows that BSFC reduces as the load increases from 19.6 Nm to 117.6 Nm. ANOVA values for BSFC analysis are tabulated in Table 7. Also, the regression model for BTE is given in Eq. (4). It is found that both input parameters significantly affect BSFC. From Figure 7, it is observed that BSFC reduces with an increase in CR and NA levels. The observed trend is in line with the trend reported in the literature (14, 22). This is because the in-cylinder pressure and combustion temperature have increased, resulting in more output power and improved fuel efficiency. Also, the increased surface area of NA induces fuel oxidizer contact resulting in reduced BSFC.

3.2 Interpretation of Machine Learning Results

The comparison of the outcomes obtained from our methodology with those derived from experimentation is an essential process in substantiating the efficacy of the deep learning-based surrogate model, a type of Machine Learning (ML) model. The objective of the present study is to address the existing disparity by offering improved solutions that are both efficient and accurate. This comparative analysis aims to evaluate the extent to which our deep learning model accurately replicates the BTE and BSFC projected by experimentation. From the comparison, it is confirmed that the present methodology exhibits a strong correlation with experimental results while substantially decreasing computing time, it not only confirms the viability of using deep learning in this domain but also emphasizes the possibility of achieving quicker and more economical analysis. Furthermore, doing such a comparative analysis will provide valuable insights into the strengths and weaknesses of each methodology, hence guiding forthcoming determinations and influencing the integration of state-of-the-art technologies within the realm of fuel analysis.

Figure 8 displays the evaluation metrics for three trained models on the test data set. All models are trained using the same 7500 training dataset and evaluated using the 2711 test dataset. The accuracy of the deep learning model was much higher (94%) compared to other models such as Random Forest (72%), Decision Tree (60%), Support Vector Machines (55%), Gradient Boost Regressor (50%), and K-Nearest Neighbor (40%). Thus, the deep learning model outperforms both Random Forest and Gradient Boost-based Regressor in all evaluation metrics. Convincing results are obtained while comparing models based on MAE and RMSE.

Table 6. ANOVA for BTE

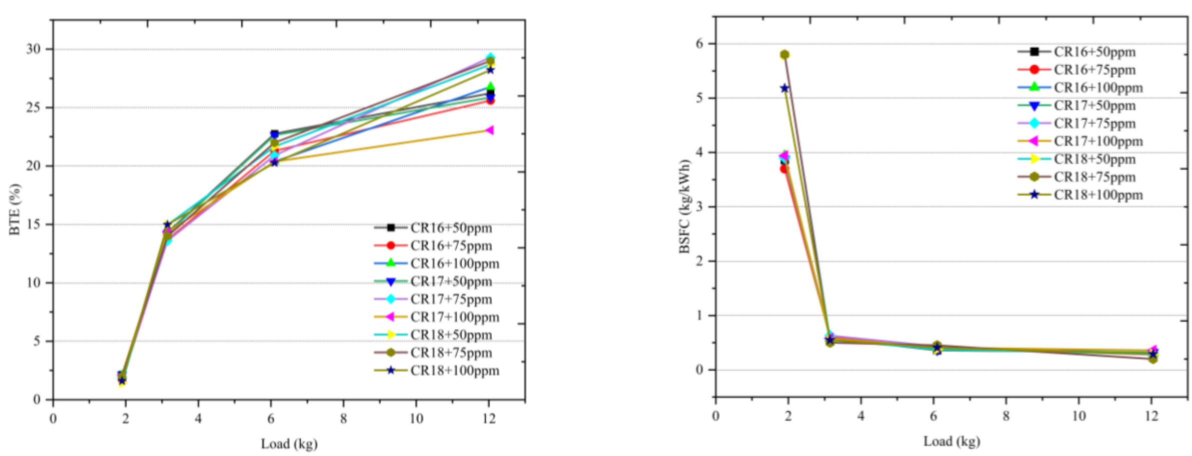
Source	Sum of Squares	df	Mean Square	F-value	p-value
Model	4.84	5	0.9672	96.05	0.0017
A-Compression ratio	3.3	1	3.3	327.74	0.0004
B-Nanoparticles	0.1262	1	0.1262	12.53	0.0384
AB	0.0625	1	0.0625	6.21	0.0884
A²	0.8235	1	0.8235	81.77	0.0029
B²	0.5236	1	0.5236	51.99	0.0055
Residual	0.0302	3	0.0101		
Cor Total	4.87	8			

$$BTE = 196.757 - 20.7\times A - 0.032\times B - 0.005\times A\times B + 0.6416\times A\times A + 0.0008\times B\times B \quad (3)$$

Table 7. ANOVA for BSFC

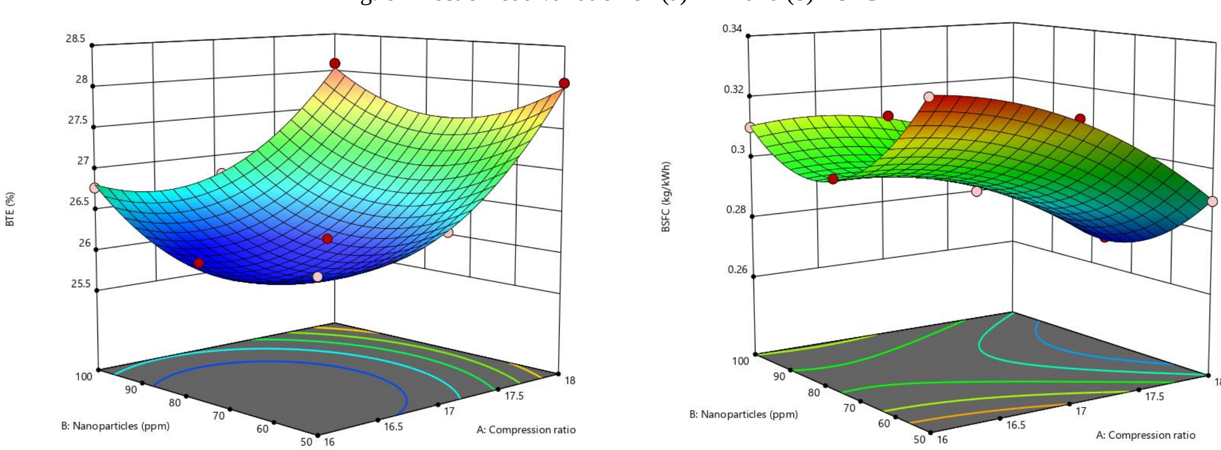
Source	Sum of Squares	df	Mean Square	F-value	p-value
Model	0.0027	5	0.0005	224.47	0.0005
A-Compression ratio	0.0014	1	0.0014	569.53	0.0002
B-Nanoparticles	0.0002	1	0.0002	63.28	0.0041
AB	0.0001	1	0.0001	42.19	0.0074
A²	0.0002	1	0.0002	63.37	0.0041
B²	0.0009	1	0.0009	384	0.0003
Residual	7.11E-06	3	2.37E-06		
Cor Total	0.0027	8			

$$BSFC = -1.494 + 0.264\times A - 0.0002\times B - 0.008\times A\times B - 0.008\times A\times A + 0.000034\times B\times B \quad (4)$$



(a) (b)

Fig. 6 Effect of load variation on (a) BTE and (b) BSFC



(a) (b)

Fig. 7 Effect of Compression ratio and Nanoparticle additives on (a) BTE and (b) BSFC

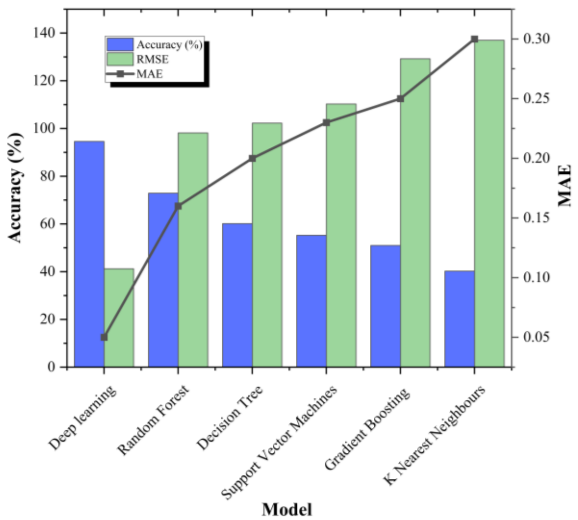


Fig. 8 Comparison of Accuracy and Error Metrics for different models

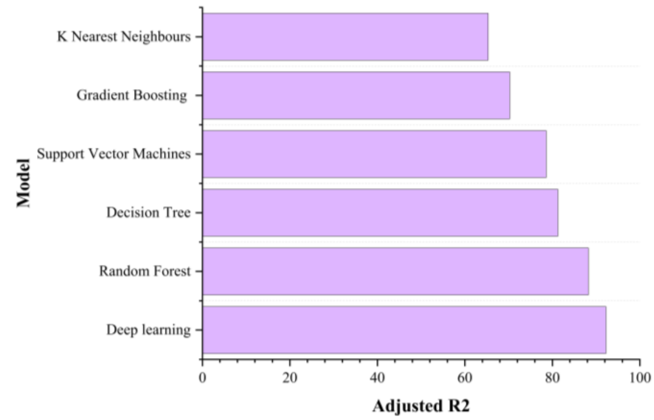
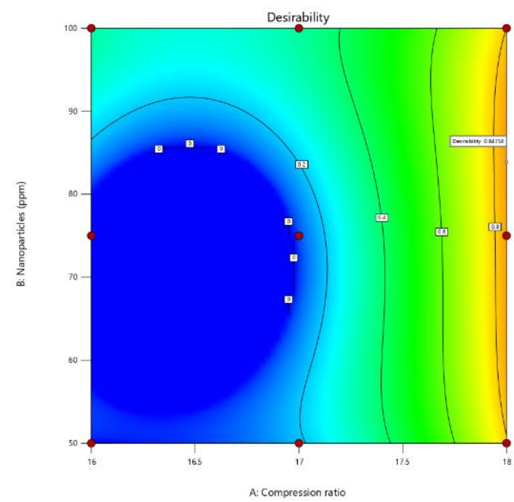
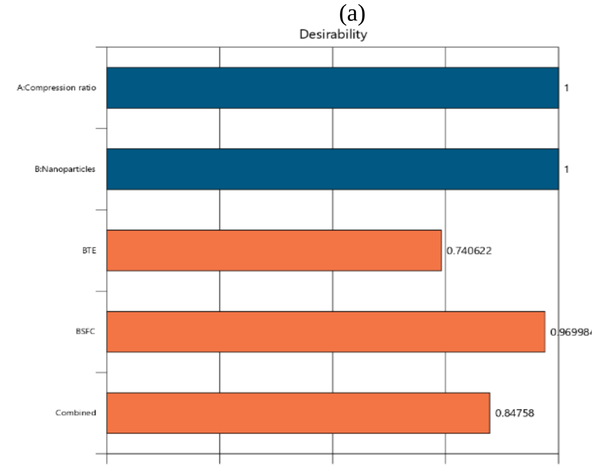


Fig. 9 Comparison of Adjusted R2 for different models



(a)



(b)

Fig. 10 Desirability (a) Contour plot and (b) Bar graph

One of the key aspects that distinguishes the present study is the integration of ML techniques to analyze the performance of cerium oxide blended biodiesel, particularly fuel consumption metrics such as BSFC. ML plays a pivotal role in extracting meaningful insights from complex datasets, especially in domains where traditional analytical approaches may fall short. In the context of the present study, the utilization of ML algorithms facilitates:

1. Pattern Recognition and Prediction: By training models on historical data comprising various operational parameters and corresponding performance metrics, ML algorithms can effectively recognize patterns and predict future outcomes. In our case, these models can predict BSFC values under different operating conditions, aiding researchers and research and development (R&D) engineers in understanding the fuel consumption behaviour of cerium oxide blended biodiesel across a wide range of scenarios.

2. Optimization and Decision Support: ML algorithms can be further leveraged to optimize engine performance and guide decision-making processes. Through iterative learning and optimization techniques, these algorithms can identify optimal operating conditions that minimize fuel consumption while maximizing efficiency and performance. This aspect is particularly valuable for researchers and R&D engineers involved in the development and optimization of biofuel formulations and engine systems.

3. Insight Generation: Beyond mere prediction and optimization, ML enables the generation of actionable insights from complex datasets. By analyzing the relationships between input parameters and performance metrics, these algorithms can uncover underlying trends, correlations, and causal relationships that may not be readily apparent through traditional analysis methods. Such insights are instrumental in guiding further research directions, refining experimental protocols, and informing strategic decisions in biofuel development and engine design.

In summary, the incorporation of ML in the present study offers several tangible benefits to researchers and R&D

engineers engaged in the development and optimization of cerium oxide blended biodiesel and associated engine systems.

In the present study, another metric for evaluating models is considered, namely Adjusted R^2. Adjusted R^2 is a valuable measure for model evaluation as it increases only when an added variable significantly improves the model. Consequently, Adjusted R^2 accounts for only significant independent variables. Figure 9 displays the Adjusted R^2 graph for various models, indicating that the highest value of Adjusted R^2 is attained with the Deep Learning model.

3.3 Optimization

The desirability function approach, a multi-objective optimization method, is used for optimization purposes. The in-built optimization module of Design-Expert 13 software is used to maximize BTE and minimize BSFC. It is observed that CR of 18 and NA level of 83.877 ppm provide optimized values of BTE as 27.583% and BSFC of 0.272 kg/kWh. The contour plot and bar graph of desirability are shown in Figure 10.

3.4 Confirmation test

Experimental confirmation tests are performed in input parameters such as CR of 17 and NA level of 75ppm to check the accuracy of developed regression models. Table 8 shows the results of the confirmation test. The error percentage is less than 5. Therefore, the developed models are satisfactory.

Table 8**.** Results of confirmation tests

Responses	Predicted	Actual	% Error
BTE	26.16	24.9	4.817
BSFC	0.291	0.302	3.78

3.5 Practical Implications

These findings represent an innovative advancement in using deep learning-based surrogate modelling to greatly improve the effectiveness of prediction, specifically in the domain of fuel analysis. The pragmatic implications of the present methodology within the industrial sector are considerable and include a broad spectrum. This study presents a good solution for numerous industries, such as petrochemical, energy, aerospace, and manufacturing, by incorporating deep learning-based surrogate modelling into fuel analysis. The accurate and efficient prediction of response characteristics is of utmost importance in ensuring the effectiveness of vital activities. Consequently, the present advancement has the potential to increase overall efficiency and dependability.

3.6 Limitations of the present study

The current study signifies a notable advancement in the use of deep learning-based surrogate modelling in the context of fuel analysis. However, it is crucial to recognize and address the inherent constraints associated with this research. The accuracy of the surrogate model is contingent upon the quality and representativeness of the training data. The use of incomplete or biased datasets might result in inferior performance of models. Moreover, it is worth noting that the deep learning model may have difficulties in extrapolating its learned knowledge to situations that are not represented in the training data. This underscores the need to have a dataset that is both varied and complete. Another constraint is the comprehensibility of the deep learning model. The opacity of deep neural networks often poses a significant obstacle in comprehending the precise rationale behind their predictions. The absence of interpretability might provide a disadvantage when conveying actionable information to engineers and decision-makers in industrial contexts.

3.7 Future Research

This study has made significant advancements in the use of deep learning-based surrogate modelling for fuel analysis and presents various promising avenues for future research. To increase the performance and generalizability of the model, it is recommended to delve into more sophisticated neural network topologies, such as recurrent or convolutional networks (34,35). Additionally, examining the advantages of transfer learning might be beneficial (36). Furthermore, enhancing the dataset by including a broader range of pressure vessel types and circumstances will enhance the model's versatility and practicality in real-world scenarios.

An area of study that shows potential is the integration of uncertainty quantification methods, which would allow engineers to get insight into the level of confidence and dependability associated with the predictions made by the model. The exploration of methods to enhance the interpretability and transparency of deep learning models, such as the incorporation of explainable AI approaches, is of utmost importance to establish confidence and foster adoption within industrial contexts (37). Moreover, it is possible to expand the scope of the study by investigating the integration of deep learning models with physics-based simulations, therefore establishing a hybrid methodology that capitalizes on the respective advantages of both approaches. This approach has the potential to provide a more comprehensive and precise resolution to intricate pressure vessel design obstacles.

Also, the increasing industrial use of deep learning in the realm of pressure vessel design necessitates more investigation into the establishment of standardized protocols and validation procedures for these models. This is crucial to guarantee their secure and dependable implementation across diverse industrial sectors.

4. Conclusion

In this study, a surrogate technique based on deep learning and RSM was employed to investigate the impact of CR and NA levels on diesel engine response. The major findings of the study are as follows:

- CR and NA levels have varied from 16 to 18 and 50 to 100 ppm, respectively. For both response characteristics, non-linear regression models have been developed, and ANOVA performed. Significant input parameters are found, and the significance level has been determined.

- Further, the input parameters are optimized to maximize BTE and minimize BSFC. The optimum operating conditions are a CR of 18 and an NA level of 83.877 ppm.
- The use of deep learning-based surrogate modelling has shown the capacity to significantly augment efficacy, enabling expedited and economically viable fuel analysis without compromising precision.
- Also, a comparison of conventional machine learning techniques with deep learning techniques has been presented based on Accuracy, MAE, RMSE, and Adjusted R^2. The study results facilitate the acceleration of design iterations and facilitate the discovery of novel insights that were previously impeded by computing limitations.
- The optimized parameters were attained at a composite desirability of 0.847. Further, confirmation experiments are performed to gauge the accuracy of the developed models.
- The obtained results from the study could help engine manufacturers predict optimal input parameters for enhanced engine performance. Future research should focus on developed fuel's long-term stability with long-term durability and endurance of engine parts.

Thus, the present study signifies a notable advancement in the field of fuel analysis.

Conflict of Interest Statement

There is no conflict of interest in the study.

CRediT Author Statement

Padmakar Kabudake: Conceptualization, Investigation,
Yashwant Kharade: Conceptualization, Writing-original draft, Validation, Supervision, Project administration
Rakhamaji Gavahane: Data curation, Formal analysis, Validation
Milind Mhaske: Formal analysis, Writing - review & editing

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