



Comparison of machine learning algorithms for predicting diesel/biodiesel/iso-pentanol blend engine performance and emissions

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ABSTRACT

In this study, machine learning techniques, namely artificial neural network (ANN), support vector machine (SVM), and extreme gradient boosting (XGBoost), were used to comprehensively evaluate engine performance and exhaust emissions for different fuel blends. To obtain valuable insights on optimizing engine performance and emissions for alternative fuel blends and thus contribute to the advancement of knowledge in this field, we focused on iso-pentanol ratios while maintaining the biodiesel ratios constant. The maximum brake thermal efficiency (BTE) values for the diesel (30.13 %), D₈₅B₁₀P₅ (29.92 %), D₈₀B₁₀P₁₀ (29.89 %), and D₇₀B₁₀P₂₀ (29.79 %) blends were achieved at 1600 rpm. At 1600 rpm, the brake-specific fuel consumption (BSFC) values for the diesel, D₈₅B₁₀P₅, D₈₀B₁₀P₁₀, and D₇₀B₁₀P₂₀ blends were 189.93, 200.93, 202.93, and 203.95 g kWh⁻¹, respectively. In engine performance prediction, the ANN model exhibited superior performance, yielding regression coefficient (R²), root mean square error, and mean absolute error values of 0.984, 0.411 %, and 0.112 %, respectively, in BTE prediction, and 0.958 %, 6.9 %, and 2.95 %, respectively, in BSFC prediction. In exhaust gas temperature prediction, the SVM model exhibited the best performance, yielding an R² value of 0.981. Although all models successfully predicted NOx emissions, the ANN model exhibited the best performance, achieving an R² value of 0.959. In CO₂ and hydrocarbon estimation, the XGBoost model exhibited the best performance, yielding R² values of 0.956 and 0.973, respectively. Therefore, the ANN model can be used to accurately predict engine performance, and the XGBoost model can be used to accurately predict emission parameters.

1. Introduction

Diesel engines find widespread use in power generation and heavy-duty transportation due to their notable advantages in terms of high efficiency, fuel efficiency, and cost-effectiveness [1]. However, these engines significantly contribute to environmental pollution and global warming by emitting greenhouse gases such as CO, CO₂, and NOx [2]. To address these concerns, alternative fuels have been developed as potential substitutes for traditional fossil fuels [3–5].

Depletion of fossil fuel resources, volatile oil prices, and stringent exhaust regulations have fueled the search for alternatives to diesel engines [6]. Biodiesel has emerged as a promising substitute due to its comparable fuel properties and reduced emissions of greenhouse gases and smoke [1,3,7]. Biodiesel, produced from vegetable and animal fats, has a similar calorific value to traditional diesel [8–10].

Vegetable and animal fats, with their higher oxygen content, lead to reduced emissions since they lack detrimental substances like

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sulfur or minerals. However, the abundance of oxygen atoms in biofuels can lead to corrosion, which is not a concern with traditional diesel fuels. Diesel fuels [1,11]. Furthermore, biofuels exhibit a higher brake-specific fuel consumption compared to conventional diesel fuels. While the presence of inherent oxygen atoms can improve exhaust emissions and combustion characteristics, it can have a detrimental impact on thermal efficiency and stability [12].

The main drawback of biofuels is increased NO_x emissions, which are the most harmful exhaust gas emissions from diesel engines [12]. As such, improving the properties of diesel and biodiesel is crucial for promoting the adoption of alternative fuels. According to Krishnakumar et al. [13], Nour et al. [14], blending high-carbon-content alcohols with diesel/biodiesel in specific proportions has the potential to enhance fuel parameters such as density, cold flow and viscosity. This research avenue can lead to more efficient utilization of alternative fuels and aid in achieving sustainable energy objectives. Combining alcohols with diesel fuel represents a promising approach to improving the properties of alternative fuels. This strategy ultimately leads to a reduction in greenhouse gas emissions and helps mitigate the negative impacts of climate change, signifying noteworthy progress within the alternative fuels domain.

The progress of alternative fuels is essential in the effort to decrease greenhouse gas emissions and tackle the issues brought about by climate change. To this end, blending alcohols with diesel fuels has emerged as a promising strategy. However, the utilization of low-carbon alcohols may influence emissions and engine performance [15–17]. In contrast, pentanol is a high-quality alcohol that can be adopted as a substitute for traditional fuels. Although extensive research has been conducted on other derivatives of pentanol, few studies have focused on iso-pentanol in diesel–biodiesel blends. As such, further research on the inclusion of iso-pentanol in fuel blends can offer valuable insights for the development of more efficient and sustainable alternative fuels. This research holds particular relevance in the ongoing pursuit of sustainable energy solutions.

The costs and time commitments associated with experimental engineering research have led researchers to explore ways to reduce the number of experimental trials [18]. Although experimental and numerical tests provide valuable insights into the effect of biodiesel fuel blends on engine performance and emissions, these methods often require considerable time and financial resources. Alternatively, modeling simulations provide a more streamlined approach for understanding the performance parameters of fuel blends, their effects on engine operation, and exhaust emissions. Among modeling methodologies, machine learning (ML)-based methods stand out as the most widely employed approach for simulations.

The primary objective of ML is to construct computational models with self-learning capabilities and data access, focusing on identifying the most effective algorithm for deriving solutions from the provided input [19]. Through autonomous learning and experience-driven improvements without explicit programming needs, ML embodies an artificial intelligence (AI) application capable of constructing predictive and interpolative models for control outcomes efficiently with increased probability. Engine performance and emissions modeling by using AI constitute an adaptable model framework that is inherently resilient to data marked by significant observed uncertainty, thus, positioning AI as a valuable tool for predicting and optimizing engine performance and emissions [15, 20–22].

ML algorithms have been employed to analyze engine performance and emissions of different fuels. Yıldırım et al. [23] compared the prediction effectiveness of support vector regression (SVR) and artificial neural network (ANN) techniques regarding engine response to different hydrogen gas fuels and found that ANN exhibited a lower total mean absolute percentage error (MAPE) than SVR, with an average difference of 53.70 %.

Namar et al. [24] utilized eleven machine learning-based regression models to construct a rapid and accurate model for predicting ignition onset in homogeneous charge compression ignition engines fueled by methane. Their findings highlighted the ML-based models' commendable response times, thus indicating their suitability for real-time applications in engines, including electronic units. Addressing the urgent requirement to mitigate the adverse impact of emissions from diesel engines on both the environment and human health, Dhahad et al. [25] proposed an AI-driven method for forecasting engine efficiency, exhaust emissions, and combustion properties of internal combustion diesel engines.

Aydın et al. [1] utilized artificial neural networks (ANN) to simulate the impact of biodiesel/diesel mixtures on engine performance and emissions. They demonstrated the ANN effectiveness in accurately predicting various performance and emission parameters, achieving high regression coefficients (R^2) ranging from 0.8663 to 0.9858. In addition, the maximum mean relative error remained below 10 % when compared with experimental results. Wang and Zhao [26] demonstrated the potential of ML algorithms in predicting fuel consumption in mining trucks. They reported that extreme gradient boosting (XGBoost) is suitable for forecasting fuel consumption in the mining sector due to its high computational efficiency and impressive prediction accuracy.

Numerous studies have explored the impact of various biodiesel blends on engine performance and emissions using machine learning (ML) techniques. However, there is a notable lack of research that directly compares the effects of different alcohol blends within a consistent biodiesel mixture on engine performance and emissions, specifically utilizing ANN, support vector machine (SVM), and XGBoost ML algorithms.

In this study, I aimed to model and predict engine performance and emissions in a 4-cylinder diesel engine by using ML algorithms. We focused on analyzing different iso-pentanol blends, keeping biodiesel blends constant. However, comparative studies on different ML algorithms, such as ANN, SVM, and XGBoost, for engine performance and emissions in the context of diesel–biodiesel–iso-pentanol blends at different ratios are lacking. In this study, we aimed to bridge the research gap by assessing the effectiveness of different ML methods in predicting engine performance and emissions under different fuel blends.

2. Materials and methods

2.1. Biodiesel production

Biodiesel was produced from safflower oil by using the transesterification method. Safflower (linas variety) oil methyl ester (biodiesel) production was performed in a programmable control device (PLC)-supported pilot production plant at Selçuk University, Faculty of Agriculture, Department of Agricultural Machinery and Technologies Engineering under the DPT 2004/7 project [27].

To produce biodiesel, 20 % crude safflower oil was mixed with methyl alcohol (CH₃OH) at a ratio of 3.5 g/L of oil to produce methoxide. This mixture was heated to 55 °C, and methoxide was added. After stirring for 60 min, glycerol in the oil was allowed to precipitate for 8 h and then separated. The methyl alcohol remaining in the crude biodiesel was removed by increasing the temperature to 75 °C. A wash was applied at 55 °C, and ash was separated from methyl ester. Finally, the samples were heated to 100 °C to obtain biodiesel [28].

2.2. Test fuels and their properties

Blended fuels were obtained by mixing safflower biodiesel, diesel, and iso-pentanol, which is a high alcohol. In these fuel blends, biodiesel content was maintained at 10 %, and iso-pentanol was blended at concentrations of 5 %, 10 %, and 20 % to produce three fuel blends. For convenience, diesel fuel is denoted as “D,” safflower biodiesel as “B,” and iso-pentanol as “P.” The blending ratios are represented as subscripts below these symbols.

In this study, kinematic viscosity, the density, water content, flash point, calorific value, and cold filter plugging point of the blended fuels were measured (Table 1).

2.3. Engine tests

The performance of engines and the emission parameters of diesel, safflower biodiesel, and blended fuels were evaluated through engine testing by using an established test setup in the Department of Agricultural Machinery and Technologies Engineering, Faculty of Agriculture, Selçuk University. The engine specifications are presented in Table 2. The engine tests were conducted according to the TS 1231 specifications (Internal Combustion Engine Test Code).

Real-time measurements were recorded for speed, torque, power, fuel consumption, oil pressure and temperature, coolant entry and exit temperatures, coolant flow speed, and exhaust gas temperature (EGT). The data were automatically transmitted to the computer by the test setup. The components of the engine test bench and their connections to the engine are illustrated in Fig. 1. The test bench comprises an engine, a hydraulic dynamometer, a magnetic pickup device, a fuel gauge, and a control unit.

The load and power values of the engine were used to calculate the BSFC and BTE, which were used as the engine performance evaluation indicators. A hydraulic dynamometer with a brake torque range of 0–400 Nm was used. BSFC was calculated using Eq. (1) [26]:

$$BSFC = \frac{\dot{m}_f \cdot 1000}{P_e}, \quad (1)$$

where *BSFC* is the brake-specific fuel consumption (g/kWh), \dot{m}_f is the hourly fuel consumption (kg/h), and P_e is the effective engine power (kW).

BTE was calculated using Eq. (2) [26]:

$$BTE = \frac{P_e \cdot 3600}{\dot{m}_f \cdot LHV} 100, \quad (2)$$

where *BTE* is the thermal efficiency (%), and *LHV* is the lower heating value (kJ/kg) of the test fuels.

An exhaust gas emission device by Mobydic was used in this study to measure emissions. This device can measure CO₂ emissions in the range of 0%–20 %, NO_x emissions in the range of 0–5000 ppm, and hydrocarbon (HC) emissions in the range of 0–20000 ppm.

Calibration accuracy, environmental conditions, inconsistency in recording observations and data processing, and the use of multiple testers result in various errors. Therefore, in this study, the uncertainty analysis method proposed by Holman [29] was used.

Table 1
Characteristics of fuels.

Fuel Characteristic	Diesel	D ₈₅ B ₁₀ P ₅	D ₈₀ B ₁₀ P ₁₀	D ₇₀ B ₁₀ P ₂₀	Standard
Density (kg m ⁻³) (15 °C)	830	832.2	831.5	829.2	EN ISO 3675 EN ISO 12185
Kinematic viscosity (mm ² s ⁻¹) (40 °C)	3.02	2.97	2.93	2.8	EN ISO 3104
Flash point (°C)	68	50	49	48	EN ISO 2719 EN ISO 3679
Water content (mg kg ⁻¹)	40.05	142	305	318	EN ISO 12937
Calori value (MJ kg ⁻¹)	10806	10578	10441	10161	DIN 51900
Cold filter plugging point (°C)		-16	-15	-14	EN ISO 3015 EN ISO 3016

Table 2
Technical specifications of the diesel engine used in this study.

Brand and model	Tümosan 4DT-39T-185C
Rated Power @2300 rpm	85 HP
Maximum torque	340 Nm
Total Engine Capacity	3908 cm ³
Diameter Stroke	104 mm × 115 mm
Number of Cylinders	4
Minimum Specific Fuel Consumption	160-g HPh ⁻¹
Aspiration	Turbocharger
Number of Valves Per Cylinder	2
Compression Ratio	17:01
Combustion System	Direct Injection
Cooling system	Water -Cooled

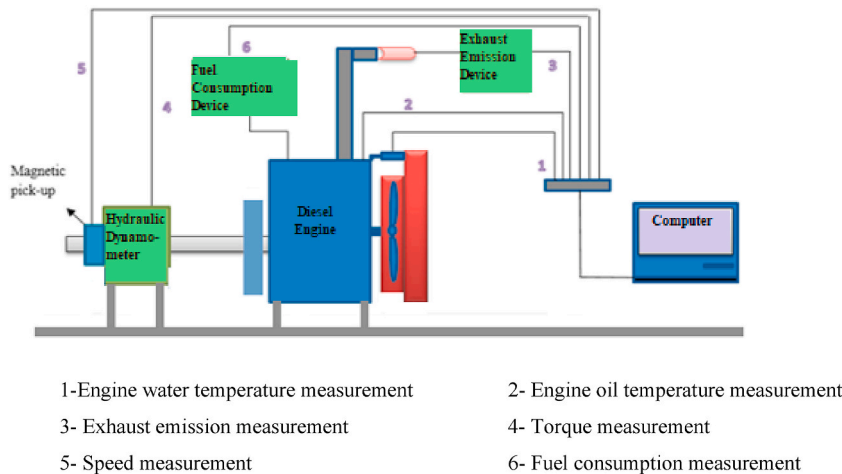


Fig. 1. Schematic of the engine test setup.

The uncertainty analysis results are presented in [Table 3](#). The overall uncertainty of the experimental setup is ± 4.29 , which is acceptable for the testing process, and the total uncertainty of the system is within acceptable limits.

2.4. ML

We performed an in-depth analysis of three ML algorithms: ANN, XGBoost, and SVM. RStudio version 2022.02.0 was used to run all three algorithms, and the models' parameters were tuned using a grid search approach. These ML algorithms were employed to predict engine response variables, namely brake-specific fuel consumption (BSFC), brake thermal efficiency (BTE), EGT, HC emission, nitrogen oxides (NO_x) emission, and carbon dioxide (CO₂) emission. Two inputs were used in the training process: engine speed (1100–2400 rpm at intervals of 100 rpm) and test fuels (diesel, D₈₅B₁₀P₅, D₈₀B₁₀P₁₀, and D₇₀B₁₀P₂₀). The study dataset comprised 336 data points (84 × 4 pixels), which were divided into training (70 %) and testing sets (30 %). The subsequent paragraphs in this subsection provide brief descriptions of the three ML algorithms used in this study.

Table 3
Uncertainty analysis results for the measurement devices used in this study.

Calculated value	Unit	Uncertainty (%)
Engine torque	Nm	± 1.05
Engine Power	kW	± 1.2
Fuel consumption	gs ⁻¹	± 1.2
Specific fuel consumption	g kWh ⁻¹	± 1.5
Dynamometer	N	± 1.2
Speed sensor	rpm	± 2
CO ₂	%	± 1.2
HC	ppm	± 1.6
NO _x	ppm	± 1.6
Exhaust gas temperature	°C	± 1.5

2.4.1. ANN

An ANN is a multilayer perceptron structure comprising an input layer, one or more hidden layers, and an output layer. ANNs employ various learning algorithms, such as radial basis networks, perceptron algorithms, backpropagation, and elastic backpropagation, to update the weights between nodes and learn the relationship between input and output variables [30,31]. ANNs can differ structurally and mathematically, with differences in the number of layers and node connections. Typically, ANNs comprise an input layer, one or more hidden layers, and an output layer [31]. The weights assigned to each node reflect the importance of the signals it carries, and the information processed by each node is calculated using a specific equation [31]. An example of the structure of an ANN is depicted in Fig. 2.

In this study, a neural network structure comprising four neurons in the first hidden layer and three neurons in the second hidden layer yielded the best prediction results for all output parameters except HC. For HC predictions, a neural network structure comprising three neurons in the first hidden layer and two neurons in the second hidden layer yielded the best prediction results. The optimal neural network structure was determined using a grid search approach, where different combinations of network structures and parameters were tested, and the network structure that yielded the highest prediction accuracy on the testing dataset was selected.

First, the data for the ANN model were normalized. Different types of data normalization methods have been presented in the literature: minimum, maximum, median, sigmoid, and Z-score normalization [32]. The Z-score method creates a statistically normal distribution and shows the position of each piece of data within the standard deviation. The standard deviation shows how far the data are from the mean: a negative value indicates that the value is below the mean and vice versa [33]. The Z-score method was used in this study to standardize the data in the ANN models.

Various algorithms have been proposed in the literature for training a network and adjusting its weights. A multilayer feed-forward ANN, along with the backpropagation algorithm, was used in this study because of its ability to model problems that cannot be linearly separated [26].

2.4.2. XGBoost

XGBoost is an ML method based on the gradient boosting decision tree (GBDT) algorithm [34]. XGBoost can be applied to supervised problems, whereas the GBDT algorithm is limited to regression and classification problems. The fast and efficient implementation of XGBoost enables more agile model exploration due to its parallel and distributed processing capability. XGBoost integrates multiple sequential secondary predictors (e.g., decision trees (DTs)) to enhance the reliability of predictions regarding the analyzed system. Additional trees are created, trained, and adjusted to minimize the cumulative residual error. The ultimate prediction results from summing the forecasts generated by the XGBoost algorithm, achieved by aggregating the residual predictions calculated by each individual tree [35]. In this study, all XGBoost models were run using the xgbTree method. In the optimal models, the nrounds parameter was set as 500 for BTE, BSFC, EGT, HC, and NO_x and as 1500 for CO₂. In the models, the maximum depth was set as 2 for BTE and HC, 4 for BSFC and NO_x, and 6 for EGT and CO₂. All models were assigned an eta value of 0.3 and a gamma value of 0.

2.4.3. SVM

SVMs are widely used to model data properties and classify data by using information related to these properties [31]. SVMs employ a binary classifier for constructing a linear-separation hyperplane to classify data. The SVM algorithm family includes various techniques, including SVR, least-squares SVM, and successive projection algorithm SVM [36]. The ϵ -insensitive function and kernel function constitute the core of SVR and are used to transform data into a higher-dimensional feature space to realize nonlinear learning in the original low-dimensional space [37,38]. In this study, radial basis functions were employed for all output parameters. Consequently, the following parameters were used: gamma = 0.5 and cost = 4 for BTE and BSFC, gamma = 1 and cost = 4 for EGT, gamma = 2 and cost = 10 for CO₂, and gamma = 0.25 and cost = 2 for HC.

2.4.4. Model evaluation metrics

The models were evaluated using R^2 , root mean square error (RMSE), and mean absolute error (MAE). R^2 , RMSE, and MAE values

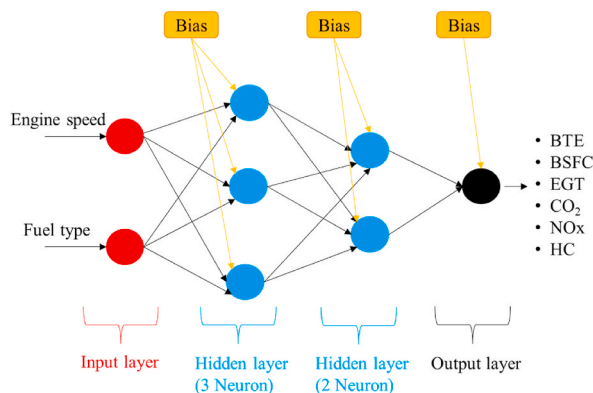


Fig. 2. Artificial neural network structure.

were calculated using Eqs. (3)–(5), respectively. The R^2 value was used for measuring model performance because it indicates the percentage of variation in the response variable that can be accounted for by the independent variables [39]. A higher R^2 value indicates a stronger predictive relationship. Conversely, the RMSE and MAE serve as measures of error, where lower values indicate better model performance [20,40].

$$R^2 = 1 - \sum_{i=1}^n \left(\frac{(o_{ei} - o_{pi})^2}{(o_m - o_{pi})^2} \right), \quad (3)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (o_{ei} - o_{pi})^2}, \quad (4)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |o_{ei} - o_{pi}|, \quad (5)$$

where n is the number of experimental data points, o_{pi} is the predicted output value, o_{ei} is the experimental output value, and o_m is the mean experimental output value.

3. Results and discussion

3.1. Engine performance

3.1.1. BTE

An illustration of the correlation between engine velocity and Brake Thermal Efficiency (BTE) is depicted in Fig. 3. The BTE of the test engine first increased from 2400 to 1500 rpm but subsequently decreased due to incomplete combustion caused by fuel accumulation in the cylinder at lower revolutions and higher engine loads [41,42]. The BTE values for all tested fuel blends ranged between 19.61 % and 30.13 %, with diesel fuel exhibiting the highest BTE. Between 1200 and 2200 rpm, all fuel blends exhibited similar trends for BTE values. At 1600 rpm, the peak brake thermal efficiency (BTE) levels achieved for diesel engines, D₈₅B₁₀P₅, D₈₀B₁₀P₁₀, and D₇₀B₁₀P₂₀ blends were 30.13 %, 29.92 %, 29.89 %, and 29.79 %, respectively. The addition of pentanol did not significantly affect the BTE of the safflower oil–biodiesel–diesel fuel blend at lower speeds (higher engine loads). According to Campos-Fernandez et al. [43], the inclusion of pentanol in diesel fuel blends did not result in any statistically significant alteration in BTE. Yesilyurt et al. [41] reported that incorporating pentanol into diesel and biodiesel fuel mixtures under high engine loads did not yield any substantial impact on BTE. Wei et al. [44] reported that increasing the proportion of pentanol in fuel blends at all engine loads resulted in a minor variation in BTE.

3.1.2. BSFC

As can be observed from the results shown in Fig. 4, the BSFC values for all test data were in the range of 189.4–291.8 g/kWh. The incorporation of iso-pentanol into the fuel blends led to an elevation in the BSFC. Ternary blends displayed a 3.9%–4.2 % rise in BSFC when compared to pure diesel. This can be ascribed to the decrease in the calorific value resulting from the heightened oxygen content in the fuel blend. As the pentanol content increases, the oxygen content in the fuel blend increases, leading to a decrease in the calorific value of the blend Yesilyurt et al. [41]. Furthermore, the aforementioned authors suggested that additional fuel must be injected to attain the same engine power when using alcohol blends. Yesilyurt et al. [41], Kumar et al. [45], Yilmaz and Vigil [46] also reported similar findings. Similarly, Campos-Fernandez et al. [43], Wei et al. [44] found that an increase in the pentanol ratio increased the

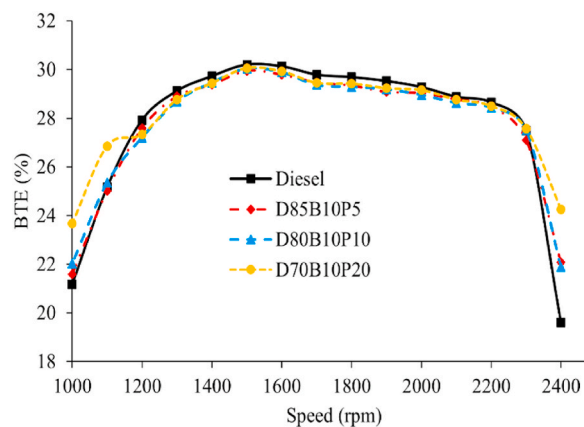


Fig. 3. Changes in BTE value for diesel and fuel blends at different engine speeds.

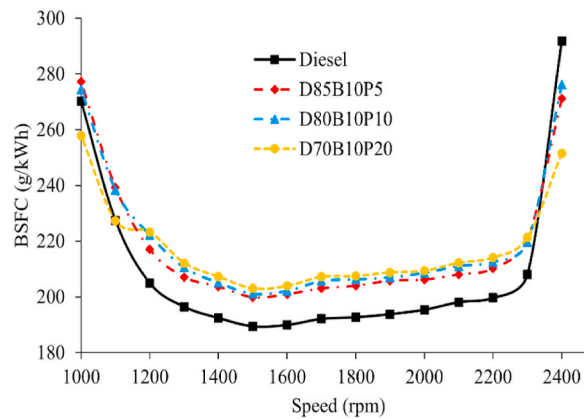


Fig. 4. Changes in the BSFC value of diesel and fuel blends at different engine speeds.

BSFC values of pentanol–diesel fuel blends, consistent with the current study. Moreover, Yilmaz and Atmanli [47] observed an increase of 5.27%–8.61 % in BSFC values when pentanol was added to biodiesel–diesel fuel blends when compared to pure diesel.

3.2. Exhaust emissions

3.2.1. EGT

The alterations in EGT for diesel fuel and triple blends of biodiesel, pentanol, and diesel are illustrated in Fig. 5a. The increase in EGT is due to a reduction in engine speed and a corresponding increase in engine load, which in turn leads to an increased amount of fuel injected into the combustion chamber, ultimately increasing the in-cylinder temperature Ong et al. [48]. The average EGT values for the diesel fuel and its blends, namely D₈₅B₁₀P₅, D₈₀B₁₀P₁₀, and D₇₀B₁₀P₂₀, were 568 °C, 553 °C, 552 °C, and 530 °C, respectively. The slightly elevated volatility and enhanced air mixture in diesel fuel result in a slightly greater peak rate of heat release compared to biodiesel blends [49]. Another contributing factor to the increased exhaust emissions from diesel fuel is the higher ignition delay encountered in diesel combustion. This prolonged ignition delay brings results in a higher quantity of fuel accumulation within the combustion chamber, ultimately increasing the peak heat release rate [49].

When the amount of iso-pentanol in the fuel blends was increased, a reduction in EGT was observed. This can be attributed owing to

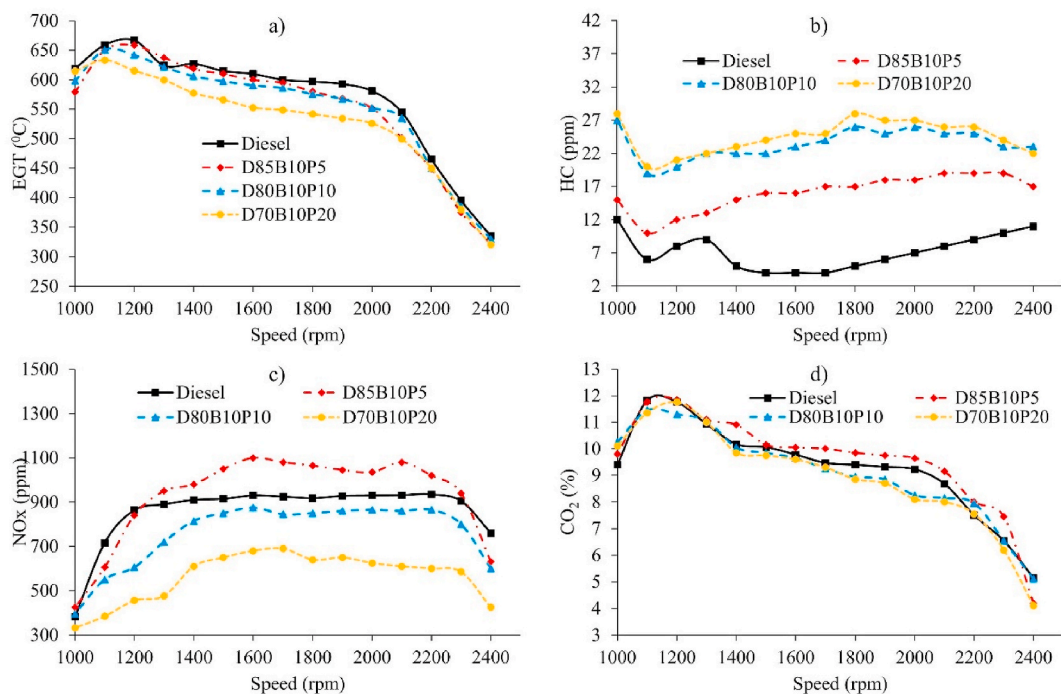


Fig. 5. Changes in (a) EGT, (b) HC, (c) NO_x, and (d) CO₂ values for diesel and fuel blends at different engine speeds.

alcohol's low calorific value, high oxygen content, and greater heat of vaporization [48,50]. Researchers such as Yilmaz and Atmanli [47], Atmanli [51], Yasin et al. [52] reported similar results, highlighting the role of high oxygen content in alcohol in reducing EGT. Furthermore, Cheung et al. [53] stated that the low calorific and high latent heat of vaporization of alcohol contribute to the reduction of EGT in alcohol blends.

3.2.2. HC emission

The HC emission variations for diesel fuel and ternary blends are shown in Fig. 5b. HC emissions there was an increase in the ternary blends as iso-pentanol content increased. This can be attributed to the alcohols characterized by a low cetane number and a high heat of evaporation, which compromise the auto-ignition characteristics of the blends. Consequently, the HC emissions increase due to the quenching effect occurring in the lean-blend region of the cylinder. This observation is in line with that presented in a previous study [54] and is consistent with previous investigations by Kumar and Saravanan [55], Nanthagopal et al. [56], Rajasekar [57], who recommended the use of high-carbon alcohols at lower blends to mitigate emissions.

3.2.3. NO_x emission

The formation of nitrogen oxides (NO_x) is primarily due to high in-cylinder temperatures and pressures [58,59]. The NO_x emission variations for diesel and ternary fuel blends are shown in Fig. 5c. The average NO_x concentrations for the diesel fuel and ternary blends with D85B10P5, D80B10P10, and D70B10P20 compositions were measured at 856, 923, 757, and 561 ppm, respectively. The reduction in NO_x emissions in fuel mixtures was found to be directly proportional to the increase in the iso-pentanol ratio. This can be attributed to the increased oxygen content and decreased calorific value caused by the incremental ratio of iso-pentanol. Çelik et al. [60] reported that alcohols in fuel blends lead to a decrease in the combustion temperature in the cylinder, resulting in a substantial reduction in NO_x emissions. In addition, Mahalingam et al. [61] concluded that the addition of different proportions of pentanol to biodiesel fuel blends results in decreased NO_x emissions. Similarly, Yesilyurt et al. [41] reported that incorporating pentanol into a blend of biodiesel and diesel fuel leads to reduced NO_x emissions.

3.2.4. CO₂ emission

The average CO₂ values for the diesel, D₈₅B₁₀P₅, D₈₀B₁₀P₁₀, and D₇₀B₁₀P₂₀ fuels were 9.28 %, 9.57 %, 9.11 %, and 8.94 %, respectively. CO₂ emissions decreased with increasing alcohol content in the fuel blends (Fig. 5d). This reduction can be attributed to the lower number of carbon atoms in the molecular structure of higher alcohols compared to diesel fuels. Alcohols prevent homogenization of the fuel mixture in the cylinder, reducing the combustion rate and the time it takes for carbon and oxygen atoms to react. As a result, less CO₂ is produced in the post-combustion exhaust gas [62].

3.3. Prediction stage

We compared the performance of three ML algorithms, namely ANN, SVM, and XGBoost, in engine performance and emission predictions for different diesel and fuel blends.

3.3.1. Engine performance

A comparison of the three algorithms for BTE is shown in Fig. 6. The R² values of ANN, XGBoost, and SVM were 0.984, 0.973, and 0.676, respectively (Fig. 6a); the RMSE values were 0.411 %, 0.606 %, and 1.878 %, respectively, and the MAE values were 0.112 %, 0.291 %, and 0.975 %, respectively. The ANN algorithm exhibited the best performance, and the SVM algorithm exhibited the worst performance. The poor performance of SVM is evident in the comparison with the experimental observation (Fig. 6b). All three algorithms exhibited unsatisfactory performance in predicting the BTE value in the 1st first observation. ANN outperformed XGBoost by 1.13 % and SVM by 45.56 % in terms of R².

The statistical metrics comparing the three algorithms for BSFC are shown in Fig. 7. The R² values of ANN, XGBoost, and SVM were 0.958, 0.926, and 0.445, respectively (Fig. 7a); the RMSE values were 6.90, 7.26, and 19.97 g kWh⁻¹, respectively; and the MAE values

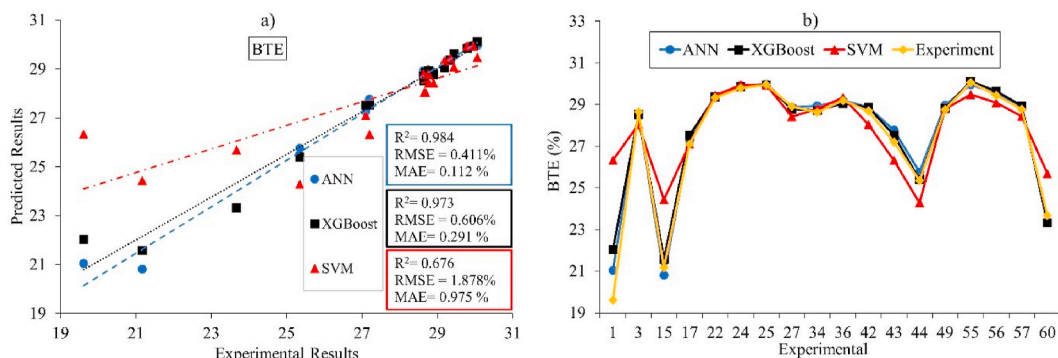


Fig. 6. a) Statistical metrics of BTE; b) Comparison of actual results and algorithm results.

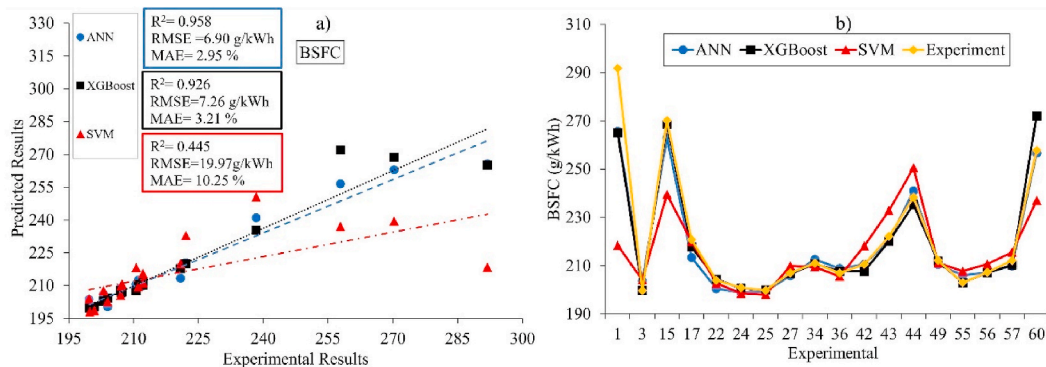


Fig. 7. a) Statistical metrics of BSFC; b) Comparison of actual results and algorithm results.

were 2.95 %, 3.21 %, and 10.25 %, respectively. The algorithms exhibited inferior performance in BSFC prediction than in BTE prediction. In BSFC prediction, ANN exhibited the best performance, whereas SVM exhibited the worst performance. As can be seen in Fig. 7b, the results of the SVM algorithm differed greatly from the experimental observations. In BTE prediction, the algorithms exhibited poor performance in predicting the first observed value in BSFC.

3.3.2. Emission performance

The R^2 values of the ANN, XGBoost, and SVM models for EGT prediction were 0.979, 0.971, and 0.981, respectively; the RMSE values were 16.68 °C, 18.5 °C, and 12.92 °C, respectively; and MAE values were 12.25 %, 14.42 %, and 9.18 %, respectively (Fig. 8a). Thus, it can be concluded that all three models performed well in EGT estimation. In terms of other error metrics, the SVM model exhibited the best performance in EGT prediction (Fig. 8b). Ağbulut et al. [2] also reported that all three models used in engine emission estimation exhibited high performance in EGT estimation.

In CO₂ emission estimation, the R^2 values of the ANN, XGBoost, and SVM models were 0.851, 0.956, and 0.861, respectively; the RMSE error metric values were 0.685 %, 0.503 %, 0.677 %, respectively; and the MAE error metric values were 0.545 %, 0.376 %, 0.504 %, respectively (Fig. 8c). Thus, it can be concluded that all three models used for estimating CO₂ emissions exhibited unsatisfactory performance, especially in the 1st and 17th observations (Fig. 8d). This was especially evident for ANN and SVM. The XGBoost model exhibited the highest accuracy in predicting CO₂ emission values.

In NO_x emission estimation, the R^2 values of the ANN, XGBoost, and SVM models were 0.959, 0.942, and 0.931, respectively; the RMSE error metric values were 48.6, 60.4, and 64.7 ppm, respectively; and the MAE error metric values were 33.54 %, 49.57 %, 39.31 %, respectively (Fig. 8e). Thus, it can be concluded that all three models exhibited satisfactory performance in NO_x estimation. However, in terms of other error metrics, the ANN model exhibited the best performance in NO_x emission estimation; moreover, all algorithms performed poorly in the 1st and 15th observations (Fig. 8f).

In HC emission estimation, the R^2 values of the ANN, XGBoost, and SVM models were 0.875, 0.973, and 0.87, respectively; the RMSE values were 2.05, 0.96, and 2.14 ppm, respectively; and the MAE values were 1.88 %, 0.76 %, and 1.98 %, respectively (Fig. 8g). XGBoost exhibited the worst performance among the three, especially in the 60th observation (Fig. 8h).

4. Conclusion

In this study, the exhaust emission characteristics and engine performance of diesel and iso-pentanol blended with safflower biodiesel were analyzed. Different modeling techniques, including experimentation, ANN, XGBoost, and SVM, were employed. The dataset was divided in the ratio of 70 %:30 % for training and testing, respectively. Fuel type and engine speed were used as input parameters, and BTE, BSFC, EGT, CO₂, NO_x, and HC were used as output parameters. The results of the study are summarized as follows:

- Increasing the iso-pentanol content in the fuel blends did not exhibit a significant effect on BTE. However, BSFC increased because of the increased amount of oxygen present in the fuel blends when the iso-pentanol ratio was increased.
- Raising the content of iso-pentanol in the fuel blends decreased the EGT.
- HC emissions in ternary fuel blends increased when the iso-pentanol ratio was increased. NO_x emissions decreased with increasing iso-pentanol concentration. A 34.4 % reduction in NO_x was observed in the D70B10P20 blend compared to diesel.
- The presence of lower carbon atom count in the composition of higher alcohols compared to diesel fuel resulted in higher CO₂ emissions. CO₂ emissions decreased with increasing the iso-pentanol ratio.
- Engine performance assessment using the BTE metric yielded R^2 values of 0.984, 0.973, and 0.676 for ANN, XGBoost, and SVM, respectively. The corresponding RMSE values were 0.411 %, 0.606 %, and 1.878 %, respectively, and the MAE values were 0.112 %, 0.291 %, and 0.975 %, respectively. Thus, it can be inferred that ANN exhibited the best performance, whereas SVM exhibited the lowest performance in BTE prediction.

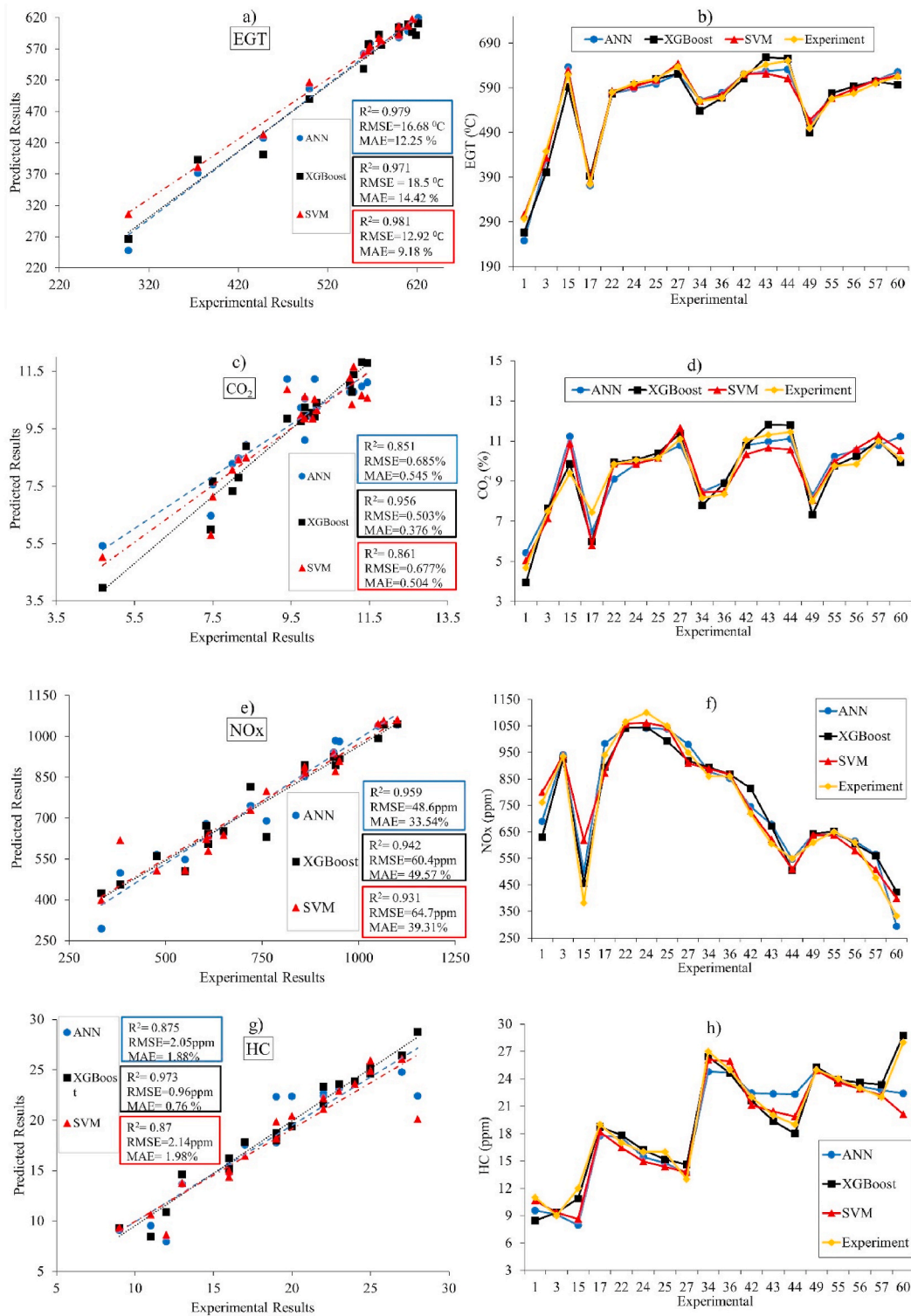


Fig. 8. Statistical metrics of emission values and comparison of actual and algorithm results.

- In BSFC prediction, ANN exhibited the best performance, whereas SVM exhibited the lowest performance.
- The models exhibited similar EGT prediction performances. However, SVM exhibited the best performance, outperforming ANN and XGBoost by 0.2 % and 1.02 %, respectively, in terms of R^2 value. A comparison of the EGT model and experimental results revealed EGT prediction models can be developed using all three algorithms; however, SVM yielded the best results.
- The XGBoost model exhibited the best performance in CO₂ and HC emission prediction. In CO₂ emission prediction, XGBoost outperformed ANN and SVM by 10.9 % and 9.93 %, respectively, in terms of R^2 . In HC emission prediction, XGBoost outperformed ANN and SVM by 10 % and 10.5 %, respectively, in terms of R^2 .
- All three models exhibited similar performance in predicting NO_x emissions. However, ANN outperformed SVM and XGBoost by 1.77 % and 2.91 %, respectively, in terms of R^2 values.
- The ANN model exhibited superior performance in predicting the engine performance parameters of fixed biodiesel and fuel blends with different diesel/iso-pentanol ratios. The XGBoost model can be used for predicting all emission parameters because it is close to the best-performing model success in EGT and NO_x emissions.
- The ANN model has excellent generalizability for accurately predicting engine performance for different fuel blends and other biodiesel feedstocks, whereas the XGBoost model has excellent generalizability for accurately predicting emission parameters.
- The effect of different iso-pentanol ratios (while keeping the biodiesel ratio constant in fuel blends) on emissions and engine performance can be modeled and predicted using ML methods.
- The experimental and numerical analyses conducted in this study offer valuable insights for researchers, scientists, and the automotive industry, and may serve as a foundation for future research aimed at devising novel methodologies or models.

To further investigate the effect of biodiesel fuel blends on engine performance and emission characteristics, in future research, we will optimize different biodiesel ratios while keeping the iso-pentanol ratio constant. In addition, we will conduct a techno-economic analysis of the current study to investigate the economic feasibility of the proposed method.

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Seda Şahin: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The author declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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