Chapter 2

Data-Driven Predictive Modeling of Cylinder Pressure: A Comparative Analysis of Gaussian Process Regression, Artificial Neural Networks, and Ensembles of Trees

Mert Gülüm[1]

Yunus Emre Karabacak[2]

Abstract

Fossil fuels have traditionally played a crucial role in global energy production, but they cause significant environmental challenges. In response, the scientific community has shifted its focus toward renewable alternative fuels. In this context, biodiesel and alcohols have emerged as promising options for diesel engines. This study is centered on predicting the cylinder pressure of a single-cylinder four-stroke diesel engine fuelled with a diesel fuel-biodiesel (methyl ester)-isopropanol ternary blend using three machine learning algorithms: Gaussian Process Regression (GPR), Artificial Neural Networks (ANN), and Ensembles of Trees (ET). The cylinder pressure data is collected under the full throttle condition and different engine speeds. GPR, ANN, and ET algorithms are trained and compared using root mean square error and regression analysis. GPR exhibits outstanding prediction performance during the validation, with a lower root mean square error of 0.12686, and r^2 of 1.00. ANN also exhibits strong prediction performance, with a validation of root mean square error of 0.47081, and a r^2 of 1.00. ET, while showing a slightly higher validation root mean square error of 1.73370, maintains strong predictive capability with an r^2 of 0.99. However, a comparison between the measured cylinder pressure data and the predicted

1 Assistant Prof. Dr., Karadeniz Technical University, Faculty of Engineering, Department of Mechanical Engineering, Trabzon, TURKEY, ORCID ID: 0000-0002-1792-3499, gulum@ktu.edu.tr

2 Assistant Prof. Dr., Karadeniz Technical University, Faculty of Engineering, Department of Mechanical Engineering, Trabzon, TURKEY, ORCID ID: 0000-0002-0268-3656 karabacak@ktu.edu.tr

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values reveals a qualitatively and quantitatively closer agreement, particularly for ANN. These findings can suggest the practicality and reliability of these algorithms for predicting cylinder pressure in internal combustion engine studies. In conclusion, this study can contribute to the expanding body of research on alternative fuels and machine learning applications in internal combustion engines.

1. Introduction

Fossil fuels currently play a crucial role in meeting a substantial portion of the world's energy demand. Given that energy constitutes a fundamental human requirement, it is anticipated that worldwide energy consumption will increase throughout the twenty-first century [1]. However, the widespread use of fossil fuels has serious drawbacks (environmental degradation, steep price increases, and the threat of fossil fuel depletion). Due to these pressing issues, the interest in alternative energy sources has experienced a significant upswing. In the current scenario, biodiesel and alcohols have garnered significant scientific interest in the recent past as renewable alternatives for diesel engines [2].

Traditionally, biodiesel is produced through a process called the transesterification (alcoholysis). This process entails the reaction of oil (triglycerides) with alcohol (generally methanol and ethanol) in the presence of a catalyst, resulting in the formation of biodiesel (fatty acid esters) and glycerol (by-product). There are a variety of catalysts available, depending on the amount of free fatty acids present in the oil, such as bases, acids, or enzymes [3].

As a renewable fuel, biodiesel is characterized by low sulfur and aromatic content, improved lubricity, higher flash point compared to diesel fuel, excellent biodegradability, and reduced toxicity [4]. It has oxygen content (10-12% by mass) within its molecular structure (thereby reducing some exhaust emissions) and good miscibility with diesel fuel [5]. In addition, biodiesel reduces net CO_2 emissions over its entire life cycle [3]. However, it has also drawbacks including increased viscosity, poor cold flow properties, lower calorific value, and reduced oxidation stability and volatility, compared to diesel fuel [4, 6].

Alcohols, a significant subset of biomass-derived fuels, have gained recognition as promising alternatives to fossil fuels. They can also serve as additives in biodiesel [7]. Isopropanol (C_3H_8O), an oxygenated additive, emerges as a significant byproduct of the IBE (isopropanol-butanol-ethanol) fermentation process. It is an isomer of propanol. The density at 293.15 K, surface tension at 313.15 K, research octane number, motor octane number, autoignition temperature, and Reid vapor pressure of isopropanol are 787 kg/m^3, 19.78 mN/m, 117, 99, 672^oC, and 9.7 kPa, respectively [8, 9]. In comparison to methanol, isopropanol exhibits lower toxicity and offers a safer option [9]. Isopropanol has a longer carbon chain than ethanol, which enhances its solubility in diesel fuel [10]. It has a slightly higher lower heating value (30.447 MJ/kg) and cetane number (12) when compared to both ethanol (~27 MJ/kg, 11) and methanol (~20 MJ/kg, 2) [8, 11, 12]. Isopropanol has a higher oxygen content (26.6%) than butanol (21.5%) and pentanol (18.15%) [11]. Isopropanol has a higher flash point (12^oC) than methanol (9^oC) [8, 11]. Isopropanol has a lower kinematic viscosity at 313.15 K (1.69 mm^2/s) than butanol (2.22 mm^2/s) and pentanol (2.89 mm^2/s) [8, 11]. Finally, isopropanol has a higher latent heat of vaporization and a lower boiling point (757 kJ/kg, 82^oC) than butanol (585.4 kJ/kg, 117^oC) and pentanol (308 kJ/kg, 138^oC) [8, 11].

For a long time, researchers worldwide have actively investigated the effects of biodiesel blends on the performance, combustion, and emission characteristics of diesel engines [13-15]. However, in recent years, machine learning methods have become increasingly prevalent in the field of internal combustion engine research, particularly in areas like optimization, predictive analysis, modeling, and fault diagnosis studies [16-20]. For example, Alahmer et al. examined the effects of adding water (5-30% wt.) to diesel fuel on brake torque and exhaust emissions of a four-cylinder four-stroke diesel engine. They used the sea-horse optimizer within the support vector regression model to determine the ideal combinations of water addition and engine speed, aiming to enhance the brake torque and reduce exhaust emissions. Moreover, a comparative analysis was conducted between the support vector regression model and the artificial neural networks model based on their performance in terms of r^2 and mean square error. The addition of 5% water, compared to diesel fuel, resulted in a 3.34% increase in brake torque. In the case of 15% water addition, the most significant reductions were obtained in CO and HC emissions, with 9.57% and 15.63%, respectively, compared to diesel fuel. NO_x emissions demonstrated an important decline, reaching a maximum reduction of 67.14% with a 30% water addition. The optimization process employing the sea-horse optimizer determined the optimal 15% water addition at an engine speed of 1848 rpm, yielding the brake torque, CO, HC, and NO_x values of 49.5 Nm, 0.5%, 57 ppm, and 369 ppm, respectively [16]. Liao et al. conducted an investigation into seven different machine learning methods (artificial neural networks, support vector machine, nonlinear autoregressive algorithm with exogeneous inputs, long short-term memory, gated recurrent unit, transformer, and temporal convolutional networks) to predict transient emissions of a diesel engine (turbocharged, common rail injection system, four-cylinder) fuelled with pure diesel fuel. These machine learning methods were assessed using evaluation metrics (r^2, mean absolute error, and root mean squared error). For the NO_X prediction, the gated recurrent unit and temporal convolutional networks models exhibited the highest accuracy. For CO and CO_2 predictions, the temporal convolutional networks and long short-term memory emerged as the optimal methods, respectively. The transformer model demonstrated relatively superior overall performance for the HC prediction. The support vector machine model, characterized by its simplicity, outperformed others in predicting exhaust pressure. Finally, a hybrid prediction model (Ensemble learning methods) was proposed, combining the best-performing algorithms for each emission characteristics parameter, resulting in an enhanced overall prediction accuracy [17]. Ramteke et al. introduced potential techniques for fault diagnosis aimed at detecting and identifying the scuffing faults in diesel engine components. They utilized condition monitoring techniques (vibration and acoustic emission analyses) for capturing signals associated with these faults. These signals were subjected to analysis in both the time-domain and time-frequency domain, employing fast Fourier transform and short-time Fourier transform methods. Moreover, artificial neural networks were used to estimate and categorize the scuffing faults. According to the results, the fast Fourier transform and short-time Fourier transform methods yielded superior fault diagnostic information [18]. Magesh et al. conducted a study to assess the effects of blends consisting of pumpkin-maize biodiesel, diesel fuel, and diethyl ether blends on the performance, combustion, and emissions of a diesel engine running at 1500 rpm under various load conditions. The addition of 5 mL of diethyl ether to 20% pumpkin-maize biodiesel-80% diesel fuel binary blend (v/v) led to a significant improvement of 31.91% in brake thermal efficiency. Furthermore, this blend resulted in reduced brake specific fuel consumption, lower HC emissions, and decreased smoke opacity, relative to diesel fuel. The study also found a 17.2% decrease in NO_x emissions at 100% load relative to diesel fuel when using a 20% pumpkin-maize biodiesel-80% diesel fuel binary blend with diethyl ether additive (5 mL). The use of artificial neural networks resulted in predicting brake thermal efficiency and NO_x emissions with r^2 values of 0.93 and 0.95, respectively. These results indicated that the artificial neural networks exhibited superior predictive capability when compared to other models (support vector regression, K-nearest neighbor algorithm, and deep learning) [19]. Murugesan et al. collected a substantial amount of data during engine testing to construct artificial intelligence-driven prediction models. They predicted the cylinder pressure of a single-cylinder diesel engine as a function of crank angle and engine load using an artificial neural networks model. The backpropagation algorithm was employed to build the prediction model. The most successful artificial neural networks of the prediction model achieved a mean square error of 0.0012, with a correlation factor of about 0.9999 for the training, testing, and validation phases. These findings illustrated the prediction model's ability to accurately anticipate cylinder pressure for any single-cylinder diesel engine [20].

Similar optimization, predictive analysis, modeling, and fault diagnosis studies can be also found in the literature [21-23], however, there also remains a substantial need for further research focused on comparing different machine learning methods in predicting cylinder pressure at reducing the time and cost associated with engine development and process improvement. Therefore, in this study, Gaussian Process Regression (GPR), Artificial Neural Networks (ANN), and Ensembles of Trees (ET) are used to estimate the cylinder pressure of a diesel engine fuelled with a diesel fuel-biodiesel (methyl ester)-isopropanol ternary blend depending on crank angle (degree) and engine speed (rpm).

2. Materials and Methods

2.1. Measurement of Cylinder Pressure

In this study, in order to measure cylinder pressure, the utilized experimental setup consists of a single-cylinder four-stroke air-cooled diesel engine, an electric dynamometer, a data acquisition system, and control panel monitoring systems. No modifications or adjustments have been made to the engine or the fuel supply/injection system. The data acquisition system comprises an engine cycle analyzer, a cylinder head pressure piezoelectric transducer (manufactured by Kistler, with a sensitivity of approximately 36 pC/bar and a measuring range of 0-300 bar), and an optical crank angle encoder with a resolution of 1 degree of crank angle. Cylinder pressure data is collected at intervals of 1 degree of crank angle. To ensure a stable operating condition at full throttle, the engine is run for a period of time before measurements are taken. The experimental data is recorded during steady-state conditions. More knowledge can be found in Refs. [24, 25]. The cylinder pressure data of the diesel engine fuelled with a diesel fuel-biodiesel (corn oil methyl ester produced by using potassium hydroxide)-isopropanol ternary blend is measured at full throttle and different engine speeds (1000-2200 rpm). For the ternary blend, a volume of 2% isopropanol is added to the binary blend including 20% biodiesel and 80% diesel fuel by volume.

2.2. GPR, ANN, and ET Algorithms

Data-driven machine learning algorithms have been widely adopted to solve a variety of engineering problems, including classification, analysis, prediction, optimization, and modeling. In this study, among these algorithms, GPR, ANN, and ET in MATLAB software (The Classification Learner Toolbox) are used for predicting cylinder pressure data depending on crank angle and engine speed. Although these algorithms are utilized for predicting continuous dependent variable values, they exhibit unique characteristics and employ distinct methodologies. To provide a comparison of GPR, ANN, and ET, Table 1 provides an overview of their features and distinctions. To guarantee the reliability and robustness of these algorithms, the input and output datasets are partitioned randomly into three distinct sets: training (70%), validation (15%), and testing (15%). The prediction performance of these machine learning algorithms is compared using two main evaluation metrics: root mean square error (RMSE) and regression analysis (r^2). A comprehensive understanding of the input and output data used for these algorithms can be seen in Table 2. In addition, Table 3 shows the hyperparameters of the machine learning algorithms used in this study.

Table 1. Some properties of GPR, ANN and ET [26, 27].

Algorithm	Advantages	Drawbacks	Use
GPR	Makes predictions with uncertainty.	Computationally expensive for large datasets.	Small to medium-sized datasets. Regression tasks. Tasks requiring uncertainty estimation.
ANN	Suitable for complex tasks.	Require large amounts of data.	Regression. Image recognition. Natural language processing.
ET	Improved generalization.	Increased complexity.	Classification and regression tasks.

Table 2. Parameters used as input and output in GPR, ANN, and ET.

Input Parameters		Output Parameter
Engine speed (rpm)	1000, 1300, 1600, 1900, 2200	Cylinder pressure (bar)
Crank angle (degree)	-180÷180	

Table 3. Hyperparameters of GPR, ANN and ET.

GPR	ANN	ET
Preset: Matern 5/2 GPR	Preset: Trilayered Neural Network	Preset: Boosted Trees
Basis function: Constant	Number of fully connected layers: 3	Minimum leaf size: 8
Kernel function: Matern 5/2	First layer size: 10	Number of learners: 30
Use isotropic kernel: True	Second layer size: 10	Learning rate: 0.1
Kernel scale: Automatic	Third layer size: 10	
Signal standard deviation: Automatic	Activation: ReLU	
Sigma: Automatic	Iteration limit: 1000	
Standardize: True	Regularization strength (Lambda): 0	
Optimize numeric parameters: True	Standardize data: Yes	

3. Results and Discussion

This section involves estimating the cylinder pressure of the diesel engine fuelled with a ternary blend of diesel fuel, biodiesel, and isopropanol by using GPR, ANN, and ET. Table 4 shows the performance indicators of GPR, ANN, and ET in predicting the cylinder pressure. Figure 1 depicts the validation and testing outcomes of these machine learning algorithms.

Table 4. Training results of GPR, ANN and ET.

Algorithm	RMSE validation	r^2 validation	RMSE test	r^2 test
GPR	0.12686	1.00	3.8126	0.96
ANN	0.47081	1.00	1.1305	1.00
ET	1.73370	0.99	0.8359	1.00

Table 4 and Figure 1 provide a comprehensive analysis of the training outcomes for GPR, ANN, and ET, emphasizing their performance across both validation and test datasets. GPR demonstrates remarkable precision in predicting cylinder pressure, with a lower RMSE of 0.12686 for the validation dataset. This signifies that GPR excels in capturing the complex relationships between input parameters (crank angle and engine speed) and output parameter (cylinder pressure). Moreover, the perfect r^2 value of 1.00 for the validation dataset showcases a flawless fit between predicted and actual values, underlining the GPR model's robustness. When evaluated on the test dataset, GPR provides adequate predictive accuracy, although RMSE increases slightly to 3.8126. However, it's important to note that this RMSE value is still quite reasonable considering the complexities of predicting cylinder pressure under varying conditions. The r^2 value of 0.96 on the test dataset further confirms an adequate correlation between GPR's prediction and the actual cylinder pressure data. Shifting the focus to ANN, we observe a validation RMSE of 0.47081, indicating well-predictive performance but slightly higher than that of GPR. However, ANN compensates with a perfect r^2 value of 1.00 for the validation dataset, signifying an excellent fit between its prediction and the actual data. On the test dataset, ANN maintains its accuracy with an RMSE of 1.1305 and an r^2 value of 1.00, underscoring its robustness and capability to predict cylinder pressure. ET, while exhibiting the highest validation RMSE of 1.73370 compared to GPR and ANN, still delivers a satisfactory predictive capability. The validation r^2 value of 0.99 indicates a high level of agreement between its prediction and the actual data. When applied to the test dataset, ET performs with an RMSE of 0.8359 and a perfect r^2 value of 1.00, demonstrating its accuracy in predicting cylinder pressure under various conditions.

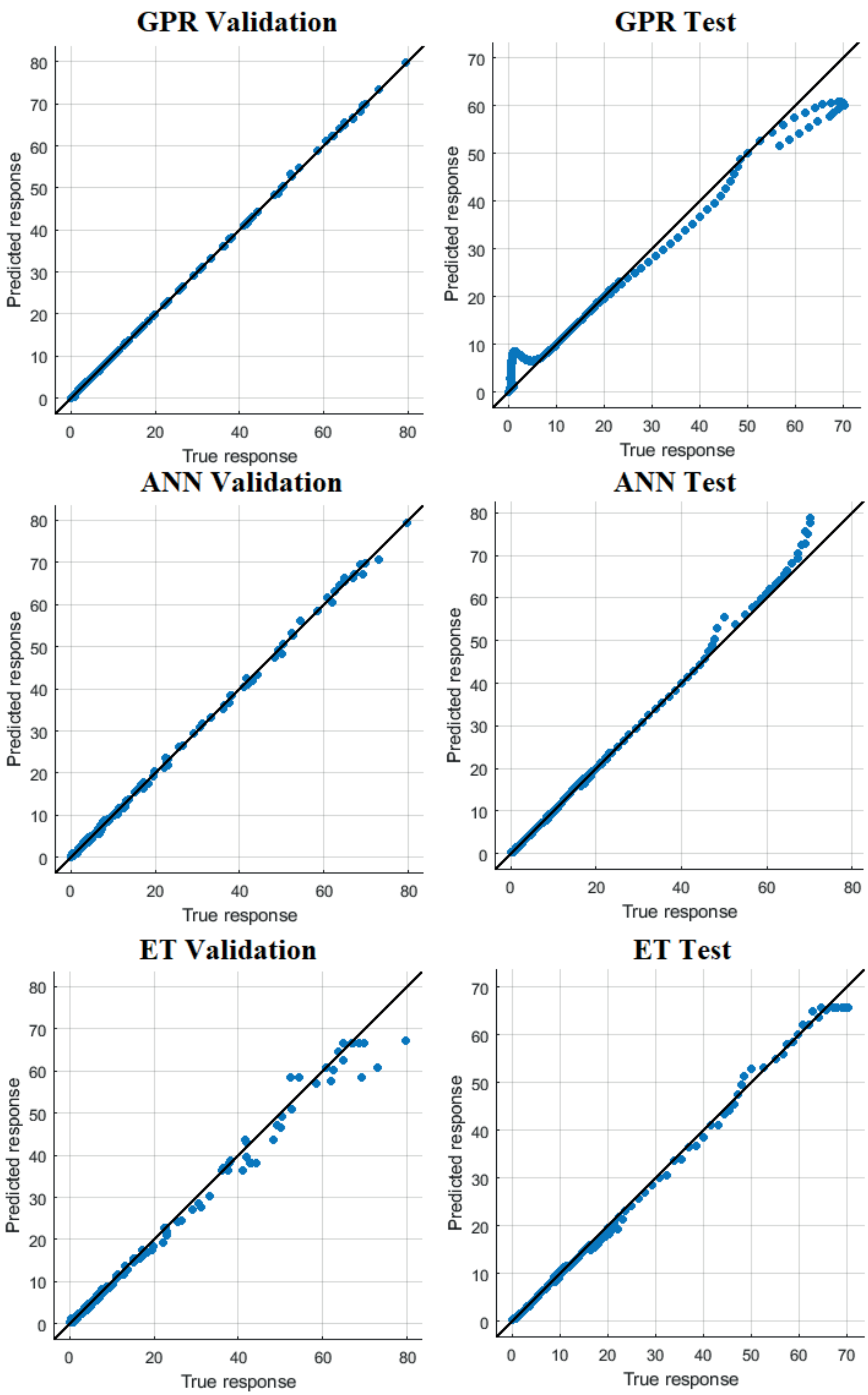

Figure 1. Validation and test results of GPR, ANN, and ET

As a result, all three machine learning models showcase promising results in predicting cylinder pressure. In particular, GPR excels in validation, while ANN and ET demonstrate remarkable fits in the test dataset. These findings emphasize the potential practicality and reliability of these models for predicting cylinder pressure across different operational conditions, which could have significant implications in various engineering applications.

Figures 2-6 illustrate the measured cylinder pressure data of the diesel fuel-biodiesel-isopropanol ternary blend at varying engine speeds, along with the corresponding predicted values from GPR, ANN, and ET. At the engine speed of 1000, 1300, 1600, 1900, and 2200 rpm, the maximum cylinder pressure is measured as follows: 79.9 bar (6 crank angle after top dead center), 78.6 bar (8 crank angle after top dead center), 70.2 bar (8 crank angle after top dead center), 69.9 bar (9 crank angle after top dead center), and 67.1 bar (11 crank angle after top dead center), respectively. With the increase of engine speed, the maximum cylinder pressure decreases since the time taken for the combustion becomes shorter and the mechanical losses increase. The crank angle location of maximum cylinder pressure moves away from the top dead center with increasing engine speed. Moreover, as shown in Figures 2-6, at 1000 and 1300 rpm, qualitatively well agreement can be observed between the measured data and estimated values from all models. However, at other all engine speeds (1600, 1900, and 2200 rpm), only ANN provides sufficient qualitative agreement with the measured cylinder pressure data.

In summary, the analysis of machine learning models (GPR, ANN, and ET) reveals ANN has qualitatively and quantitatively strong predictive capability for cylinder pressure data. This result can be attributed to the fact that the number of data, algorithm structure of ANN, and its hyperparameters given in Table 1 and Table 3 are suitable for the non-linear character of the cylinder pressure data. Finally, this study can offer practical and reliable solutions for predicting cylinder pressure under different operational conditions, which could have significant implications in various engineering applications.

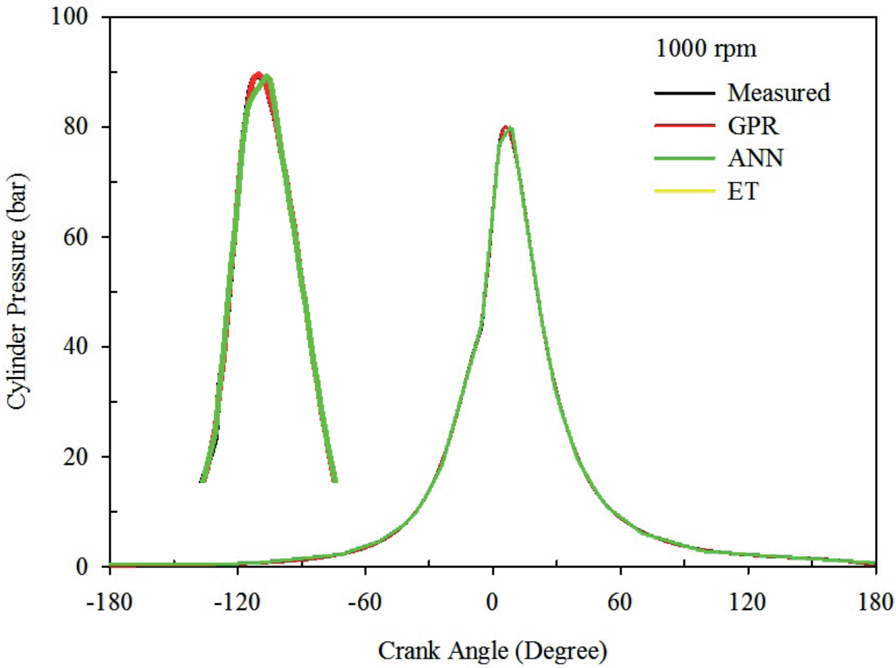

Figure 2. Comparing pressure data measured at 1000 rpm with the predicted pressure values generated from GPR, ANN, and ET

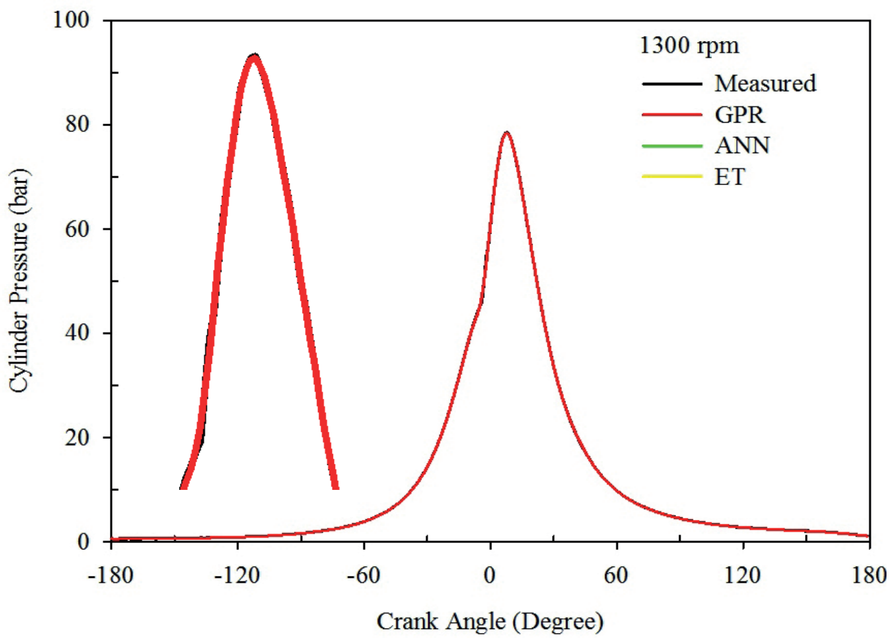

Figure 3. Comparing pressure data measured at 1300 rpm with the predicted pressure values generated from GPR, ANN, and ET

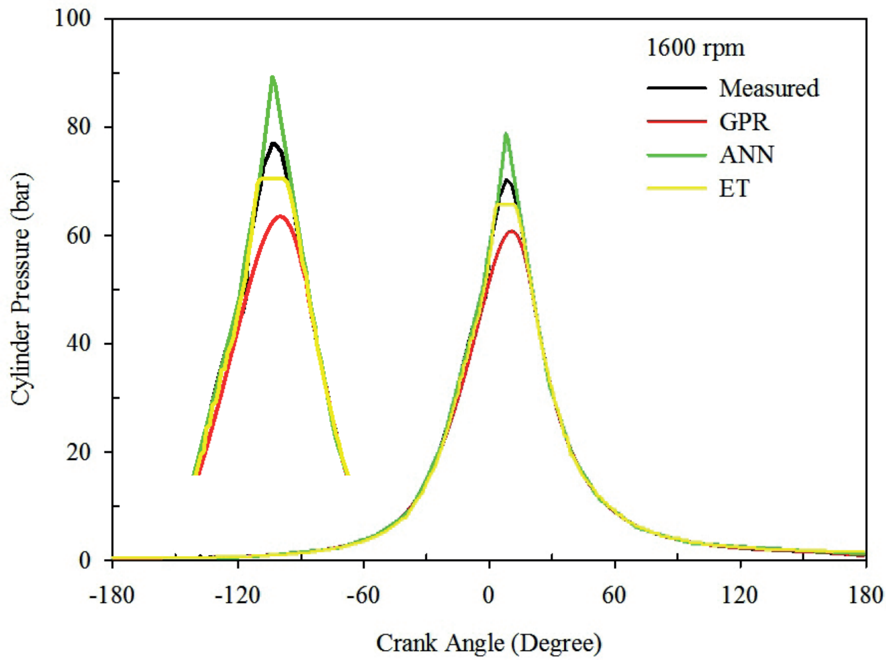

Figure 4. Comparing pressure data measured at 1600 rpm with the predicted pressure values generated from GPR, ANN, and ET

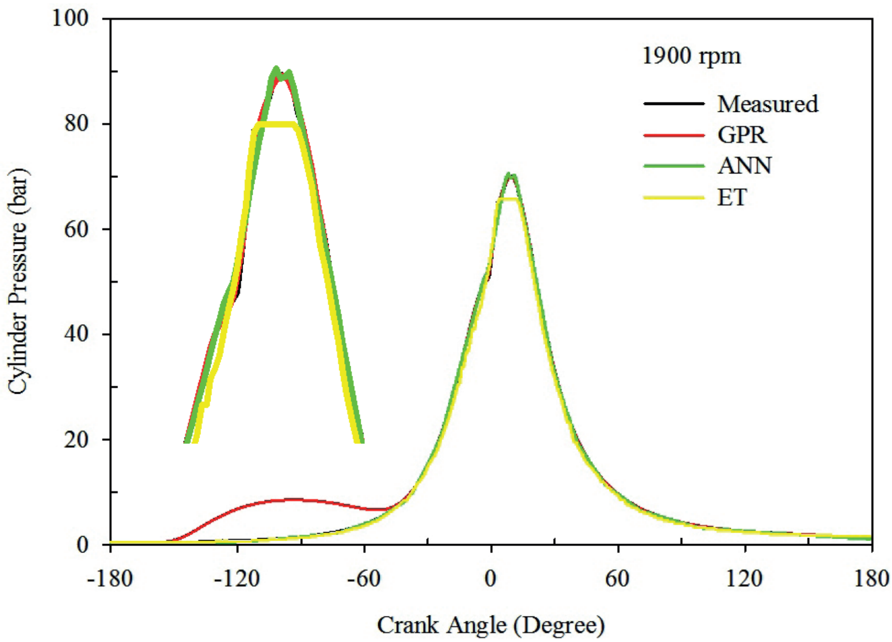

Figure 5. Comparing pressure data measured at 1900 rpm with the predicted pressure values generated from GPR, ANN, and ET

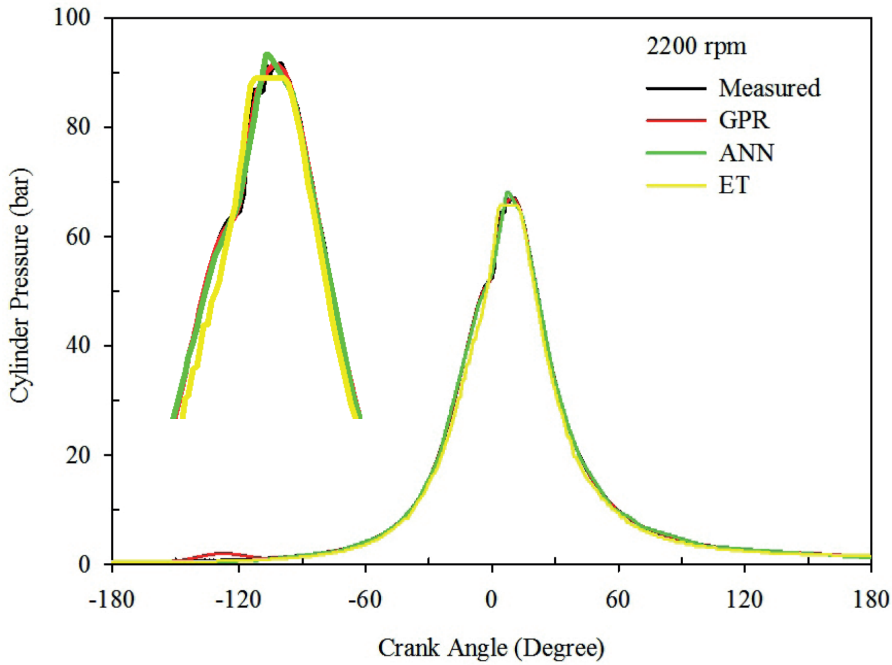

Figure 6. Comparing pressure data measured at 2200 rpm with the predicted pressure values generated from GPR, ANN, and ET

4. Conclusion

Biodiesel stands out as a promising alternative to diesel fuel due to its many advantages. Despite their low cetane number, alcohols have also arisen as promising oxygenated fuel additives for diesel engines. Researchers have long been examining the effects of diesel fuel-biodiesel-alcohols blends on the performance, combustion, and emission characteristics of diesel engines under various operating conditions. Moreover, in recent years, researchers have directed their attention toward investigations related to optimization, predictive analysis, modeling, and fault diagnosis using machine learning methods for internal combustion engines. Therefore, in this study, a number of cylinder pressure data of a single-cylinder diesel engine fuelled with a diesel fuel-biodiesel-isopropanol ternary blend are collected under different engine speeds. The cylinder pressure data collected during engine testing serves as the foundation for constructing a prediction model using machine learning methods such as GPR, ANN, and ET.

The results from GPR, ANN, and ET models demonstrate their ability to quantitatively provide promising predictions when estimating cylinder pressure. However, ANN qualitatively and quantitatively outperforms in estimating the cylinder pressure than others. In other words, compared to others, ANN shows superior accuracy as indicated by excellent fit (r^2 = 1.00) to both validation and test datasets, and the relation between cylinder pressure and crank angle (degree) is found to be more accurately described by ANN at all studied engine speeds. This result highlights ANN's predictive ability to capture complex relationships and patterns in cylinder pressure. This study can offer a valuable tool for researchers on internal combustion engines.

As a future study, alternative fuel blends (various combinations of biodiesel, isopropanol, and other potential additives), advanced machine learning techniques (deep learning methods to enhance prediction accuracy), optimization of engine parameters, the investigation of environmental impact, and economic analysis can be studied to contribute the ongoing development of cleaner and more efficient internal combustion engines.

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