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Development and Application of Artificial Neural Network for the Prediction of Engine Performance and Emission Characteristics of Diesel Engine from Fatty Acid Composition

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Abstract

The utilization of artificial neural networks (ANN) for the prediction of biofuel properties, engine performance parameters, and emission of gases within statutory regulations in engine research has been topical in recent times and is predicted to replace the cumbersome and highly technical requirements of real-time engine testing. This study developed an ANN model to predict the engine performance and emission parameters of an unmodified compression ignition (CI) engine fueled with biodiesel using two fatty acid compositions as inputs. The ANN model adopted the backpropagation with Levenberg-Marquardt algorithm, tangent-sigmoid transfer function comprising two, eight, and eight nodes as input, hidden, and output layers respectively. The overall regression coefficient (R) was found to be 0.9998 while the R-value for predicted outputs ranged between 0.9966 and 0.9997, the root mean square error varied between 0.01834 and 0.1725, and the mean absolute percentage error was reported to be between 1.6243 % and 4.546 % showing an acceptable prediction accuracy. It was found that the MATLAB NNTool is a reliable and effective tool for the prediction of engine performance parameters and emission of CI engines using two fatty acid compositions as inputs thereby minimize the time, cost, and infrastructural requirements of real-time engine test.

Keywords: ANN, engine performance, emission, FAME, prediction

I. INTRODUCTION AND BACKGROUND

The rise in population, growing depletion of crude oil deposits, constrained refining infrastructure, and environmental pollution, especially emissions from transport vehicles, has placed enormous pressure on stakeholders to develop renewable and biodegradable alternatives. This has increased research for affordable, renewable, biodegradable, and environmentally amenable options which include biofuel, hydrogen, electric cars, and vegetable oil-based fuels. Various researchers [1-5] have, in their investigations, enumerated the damaging effects of the application of petroleum-based diesel (PBD) fuel in internal combustion engines to include environmental, performance, combustion, emissions, and health effects. According to the researchers, the environmental effects include the greenhouse effect, increased global temperature, and rapid climate change. Infection and inflammation of airways, risk of asthma, bronchitis, eye irritation, and lung cancer and carcinogenic effects on humans and animals' health are some of the health effects of the use of PBD fuel. In terms of performance, PBD fuel provides incomplete combustion resulting in the emission of high volumes of carbon monoxide. Biodiesel, as an alternative fuel, has been found to offer enormous advantages such as non-toxicity, renewability, biodegradability, higher lubricity, high cetane number, high flash point, positive energy balance, low to zero sulphur, and safer handling compared to PBD fuel. However, biodiesel suffers from certain demerits including poor cold flow properties, lower volatility, higher kinematic viscosity, higher NOx emission, more prone to corrosion, damaging effects on automobile parts and concrete and auto-oxidation characteristics [6-9]. The initial challenge of high production cost is being overcome by the application of waste vegetable oil and waste animal fats as feedstock. The adaptation of waste cooking oil (WCO) has been reported to cause a 60 % to 90 % reduction in the production cost of biodiesel [10, 11].

Available statistics from the International Energy Agency [12] reveal that the current global biofuel production is not increasing rapidly enough to meet the transport biofuel consumption required as specified by the Sustainable Development Scenario (SDS). Biofuel demand in shipping and aviation has continued to increase and it is projected to triple by 2030 as shown in Fig. 1. Deliberate investment and targeted research are required in the areas of feedstock development, production infrastructure, deployment of numerical and optimization techniques in the production process, and improvement of performance and emission indices towards meeting the SDS. Meeting optimal engine performance and stringent emission requirements for compression ignition (CI) engines prescribed by regulatory bodies for CI engines fueled with fatty acid methyl ester (FAME) requires testing the fuels at various engine speeds and loads, among other parameters. This entails enormous resources, time, technicality, and personnel. One of the ways to deal with these challenges is the application of high-speed computers in numerical simulation and optimization of the production, process and utilization parameters to explore and discover optimal scenarios.

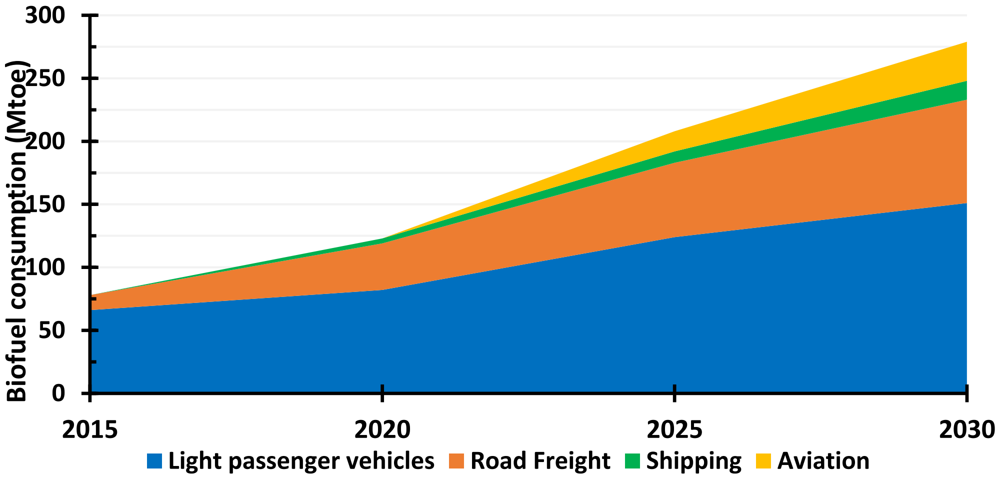

Fig. 1. Biofuel consumption breakdown in the SDS

In order to overcome the strenuous, time consuming, costly and intricate engine test experimentation involved in the determination of performance and emission parameters, researchers have adopted various numerical prediction tools to execute these important tasks. Linear prediction models have been widely used in predicting FAME properties but have been deficient in estimating engine performance and emission parameters because of their nonlinearity orientation. Artificial neural networks (ANN) have found wide application in business, medicine, engineering, image and voice recognition, with appreciable success, particularly where the traditional modeling techniques proved ineffective. ANN has been deployed for the purpose of predicting engine performance and emission of internal combustion engines [13]. An ANN uses the information presented to it to learn, relearn, and understand the correlation between the input and the output data. Using those established relationships, the ANN can predict responses from a new set of independent variables, drawing from its learning experience. A properly trained ANN possesses a high predictive capability and the ability to learn, unlearn, and relearn to improve the quality and integrity of the output if a different array of data is made available The preference of the ANN model over other prediction techniques is due to its adaptability and capability to learn then relearn nonlinear progressions and its uncomplicated adaptation to real-time data fluctuations. A well-trained ANN is faster, simpler, and more accurate than other conventional simulation techniques or mathematical models which require extensive computations, long iterations, and complex differential equations [14]. Major advantages of ANNs include high processing speed, ability to capture nonlinearities between predictors and outcomes as well as capability to learn and model linear, nonlinear, and complex correlations. Though ANNs are trained on a case by case basis which cannot be transferred for usage to other applications, this approach has continued to find applications in pattern classification, scheduling, intrusion detection, financial analysis as well as in control and optimization [15-20].

Due to its obvious benefits, researchers have employed well-trained ANN models to forecast and estimate engine performance parameters and release of emission gases on CI engines including torque, engine power, brake specific fuel consumption (BSFC), brake thermal efficiency (BTE), exhaust gas temperature (EGT), thermal efficiency, carbon dioxide (CO_2), nitric oxide (NO), nitrogen oxides (NOx), unburnt hydrocarbon (UHC), and smoke intensity under different engine speed and loading situations. The outcomes of the prediction exercises have agreed with real-time experimental engine test results, thereby meeting the primary purpose of its deployment.

Bearing in mind the importance of fatty acid (FA) composition in the handling, storage, performance, combustion, properties, and emissions of biodiesel fuel, a lot of resources and efforts are being deployed for the prediction of engine performance parameters as well as the emission based on its FA compositions. These efforts need to be improved upon and strengthened, hence the present intervention. In this research, the pertinent question to ask, and which forms the motivation for this research, is whether the numerically determined optimal FAME candidate can advance engine performance and tone down the emission characteristics of an unmodified of CI engine.

The object of the present effort, therefore, is to develop and train an ANN model with the capacity to predict the engine performance parameters and emission characteristics of an unmodified CI engine fueled with an optimal FAME candidate determined in terms of two FA compositions with the aim of unearthing an appropriate biodiesel fuel that will advance engine performance and mitigate emission characteristics. This investigation is limited to the use of C16:0 and C18:1 percentage concentrations as input variables to develop an ANN model capable of training, testing and predicting the BSFC, BMEP, BTE, EGT, CO, smoke intensity, UHC, and NOx of an unmodified CI engine fueled by unblended FAME.

The application of ANN in biofuel study has been well documented owing to the obvious derivable advantages, which include simplicity, adaptability, and maneuverability [21]. ANN has been applied on many occasions to predict biodiesel properties, engine performance, fuel mixing and combustion parameters, and emission characteristics. Filho et al. [22], Hosseinpour et al. [23], Oliveira et al. [24], and Rocabruno-Valdes et al. [25] utilized a well-trained ANN model to predict some properties of FAME. The outcome of their investigations revealed that the predicted data agreed with the experimental data. Taghavifar et al. [26] engaged ANN to predict the heat flux of a CI engine using spray characteristics such as crank angle, temperature, and pressure as inputs with acceptable output. Rao et al. [27], Javed et al. [28], and Kshirsagar and Anad [29] used ANN prediction modeling to predict BTE, BSFC, EGT, CO, CO_2, UHC, NOx, and soot using blending ratios as inputs with reasonable outputs. Çay et al. [30], and Kumar et al. [31] developed standard backpropagation algorithms on a MATLAB platform to predict the engine performance of a CI engine powered with biodiesel and compared the predicted results with experimental results. Bietresato et al. [32] evaluated the effectiveness of ANN models of sigmoidal and Gaussian algorithms to demonstrate their predictive capabilities for engine performance and emission characteristics in a farm tractor.

Other researchers have used various parameters, including temperature, number of carbon and hydrogen atoms as inputs for the prediction of properties, engine performance and emission parameters of a conventional CI engine. The use of fatty acid (FA) compositions have not been widely and adequately exploited. Ramadhas et al. [33], Filho et al. [22], Piloto-Rodriguez et al. [34], and Sara et al. [35] have at various times used FA composition as input variables to predict the properties, engine performance and emission characteristics of FAME. A painstaking and exhaustive search of literature, comprising over 120 biodiesel samples, revealed that palmitic acid (C16:0), stearic (C18:0), oleic acid (C18:1), linoleic acid (C18:2), and linolenic acid (C18:3) are the most popular FAs in biodiesel among the 13 FAs [22, 36-38]. Myristic acid (C14:0), C16:0, C18:0, C18:1, and C18:2 were adopted by Menon et al. [39] as input variables to predict various parameters of CI engine fueled with biodiesel using ANN, thereby developing an optimal biodiesel fuel candidate based of FA composition and degree of saturation/unsaturation of the fuel.

II. MATERIAL AND METHODS

In this section, we discuss the experimental and the numerical methods employed in carrying out the research. The experimental method involves the production of an optimal FAME candidate through the transesterification of waste palm oil (WPO) and the GCMS analysis of the samples to reveal the FA composition. The development and training of an ANN model to predict the engine performance and emission characteristics parameters of unmodified CI engine fueled with FAME is categorized by means of numerical techniques using advances in software computing.

II.I. Production of Optimal FAME Biodiesel from WPO and Determination of FA Composition

The WPO sample was collected from a local owner-operated restaurant at the point of disposal near the university campus while waste chicken eggshells were obtained from eateries at the University of KwaZulu-Natal, Durban, cafeteria. The waste chicken eggshells were converted to a CaO catalyst through high-temperature calcination at 900 ^{0} C as described by our earlier work [40]. The WPO was pretreated by removing food debris and moisture before subjecting it to a one stage transesterification process since the acid value was found to be 0.66 mgKOH/g.

The clean feedstock was mixed with methanol and calcined CaO catalyst in a flat-bottomed flask in the required quantity and heated on an electric cooker with a magnetic stirrer maintained at 1200 rpm while a digital thermocouple was used to authenticate the reaction temperature throughout the process. A reaction temperature of 60 ^{0} C, methanol to oil ratio of 6:1, the catalyst particle size of 75 µm, 1 % w/w catalyst: oil ratio, and total reaction time of 90 min were selected as process parameters. The ensuing mixture was subsequently filtered in a Buchner funnel filtration system assembled to retrieve the catalyst. The filtered mixture was transmitted to a separating funnel for the glycerol to coagulate at the base of the separating funnel where it was tapped off. The crude biodiesel was purified using magnesol. The purified FAME was subjected to FA characterization in a GCMS.

II.II. Development of ANN Model

ANN, available on MATLAB platform, is a parallel distributed processing computer system modeled on the functioning of the human brain with the capacity to generate, form and discover new knowledge without any help, based on the information presented to it. It comprises a number of linked and interconnected processing elements known as neutrons or nodes. The neutrons are linked with each other by synaptic weights through which signals are passed from one neuron to the other in accordance with the connecting weights. The weight of the signal is determined by the knowledge acquired in the course of the training, testing, and validation. The neutron processes information presented to it based on its dynamic state. The neuron receives input from external sources, analyzes such information, and executes non-linear operations based on it and generates an output [41, 42]. Figure 2 shows the network configuration of a typical ANN model used for this study.

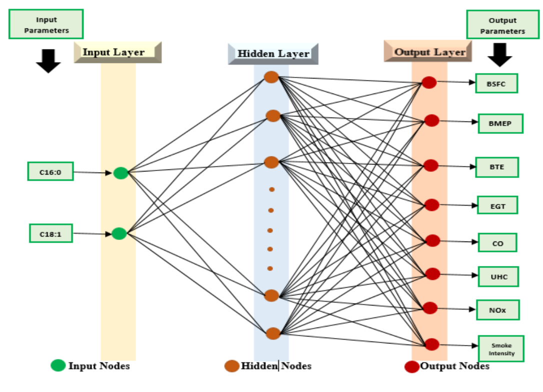

Fig. 2. The ANN structure

In order to develop and improve an ANN model, the network is exposed to the training or learning phase and the testing or validation stage. During the learning phase, the network studies the input data and estimates the output variables. In the test stage, the network stops learning and estimates the output data using the knowledge gained during the training stage. Training is programmed to terminate when the testing error attains the previously set tolerance and the preferred epoch number is reached in relation to the error value [43].

II.III. Determination of the Model Parameters

For the present research, a MATLAB R2017b NNTool was used to develop the model [44]. The back-propagation (BP) algorithm with a Levenberg-Marquardt (LM) learning algorithm was applied because of its high robustness, fault tolerance, self-learning, self-adaptability and reputation for good prediction accuracy [45, 46]. Despite this advantage, BPA has been found to be susceptible to slow convergence, fluctuations, and severe oscillations particularly during the training stage [47, 48]. Tangent-sigmoid (TANSIG) is adopted as the transfer function.

The number of nodes at the input and output layers were selected as stated on the research objective which is to use C16:0 and C18:1 as inputs to estimate the engine performance and emission characteristics of an unmodified CI engine. For this research, the selected engine performance output parameters were BSFC, BMEP, BTE, and EGT, while the emission characteristics were CO, smoke intensity, UHC, and NOx. Hence, two nodes were selected for input layers while eight nodes were selected for output layers.

A single hidden layer can sufficiently predict any non-linear relations or functions using the BPA neural network. Since there are few nodes in the input layer in the proposed model, the network did not require any complex arrangement. Hence one hidden layer was adopted for the model. The number of nodes in the hidden layer (p) was selected based on the Kolmogorov theorem and neural network theory [49]. p was estimated by Eq. 1 [50].

$$p < \sqrt{n+m} + a \tag{1}$$

Where n is the total number of nodes in the input layer, m is the total number of nodes in the output layer and a is a positive integer ($a < 10$). The a must be strategically chosen to get a reasonable p. An excessively low p will reduce the accuracy of the network approximation of the model thereby leading to increased prediction error, while an excessively large p will make the network unnecessarily complex requiring longer training time [51]. With $n\, value$ of 2, $m\, value$ of 3, and $a\, value$ of 7, p was set to 10. The learning rate and target error were both set at 0.01 based on the experience of continuous testing.

The minimum gradient of $10^{-7}$was set as part of the stopping criteria. Other factors to be considered for the design of the ANN model are depicted in Table 1. Also, as shown in Table 2, there were 125 experimental datasets mined from the literature. The FA compositions were obtained from GCMS analysis while the engine performance and emission characteristics were gotten from real-time engine tests [52-55]. 70 % (95 patterns) of the data were chosen for training the model, 15 % (15 patterns) for validation while 15 % (15 patterns) were used for testing the prediction capability of the trained network. The developed, trained, and validated model was used to predict the engine performance and emission characteristics of FAME candidates with C16:0 and C18:1 concentration of 36.4 % and 59.8 % respectively. The flow chart representing the developed ANN algorithm is shown in Fig. 3. The performance of the developed ANN model was examined by correlation coefficient (R), while the errors were evaluated using statistical error parameters, namely, Mean Square Error (MSE), Root Mean Square Error (RMSE), and the Mean Absolute Percentage Error (MAPE). The R, MSE, RMSE, and MAPE were calculated using the Eqs. 2-5 [41, 56, 57].

Table 1. Details of the neural network model

Factors	Value
Input layer	2
Hidden Layer	1
Output layer	8
Number of neutrons in the hidden layer	10
Number of epoch	10000
Number of iterations	69

$$\mathrm{R} = 1 - \left\{\frac{\sum_{i=1}^{n}(A_t - F_t)^2}{\sum_{i=1}^{n}(F_t)^2}\right\} \tag{2}$$

$$\mathrm{MSE} = \frac{\sum_{i=1}^{n}(A_t - F_t)^2}{n} \tag{3}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(A_t - F_t)^2}{n}} \tag{4}$$

$$MAPE = \frac{\sum_{i=1}^{n}\left|\frac{A_t - F_t}{A_t}\right|}{n} \times 100\ \% \tag{5}$$

Where 'n' is the number of the patterns in the dataset, 'A_t' is the actual output, and 'F_t' is the predicted output value.

The R, MSE, RMSE, and MAPE were applied to measure the accuracy of the model. The ANN model was set to terminate the iteration when $R > 98, MSE\ < 0.001, and\ MAPE < 5\ \%$. The RMSE measures the variation between the predicted data and the experimental data while the MSE denotes the standard deviation of the difference between the predicted value and the experimental value for the data. A smaller RMSE symbolizes accurate outputs and model.

Table 2. Datasets for the ANN model

S/N	C16:0	C18:1	BSFC (g/kWhr)	BTE (%)	EGT (^{0} C)	BMEP (bar)	CO (%)	Smoke intensity	NOx (ppm)	UHC (ppm)
1	20.8	58.4	266.13	33.8	408	11.92	0.07	40	451	43
2	24.5	62.6	233.31	38.58	398	12.31	0.058	43	750	55
3	31.4	58.4	325.67	27.62	466	8.91	0.026	50	543	40
4	30.6	60.3	285.14	31.55	483	9.27	0.023	56	723	35
5	21.9	57.4	280.47	32.08	449	11.15	0.21	60	468	20
6	36.3	58.4	252.18	35.68	468	11.79	0.21	54	483	34
7	23.4	70.3	231.96	38.79	400	12.17	0.069	55	459	40
8	34.5	68.4	310.43	28.98	477	9.22	0.21	58	425	50
9	36.5	57.6	272.59	33.12	459	11.64	0.049	49	471	55
10	35.6	62.4	294.53	30.55	497	10.08	0.018	42	455	53
11	34.8	60.7	257.24	34.97	430	11.38	0.04	54	460	45
12	35.8	59.3	229.81	39.15	396	12	0.07	62	446	43
13	28.5	70.6	278.83	32.27	437	10.62	0.16	66	465	50
14	43.6	56.2	255.79	35.17	431	12.17	0.032	43	675	32
15	34.8	55.9	230.03	39.11	389	12.31	0.07	45	447	34
16	26.4	65.4	279.63	32.17	494	10.9	0.13	56	456	18
17	23.6	65.3	242.07	37.17	434	12.25	0.032	48	467	32
18	26.1	65.8	226.24	39.77	388	12.39	0.01	39	478	28
19	26.7	56.5	246.55	32.43	380	12.67	0.06	30	290	34
20	34.6	54.2	246.78	40.43	342	10.56	0.05	58	875	32
21	34.3	51.6	355.74	32.76	250	9.65	0.03	62	650	28
22	24.5	49.5	290.52	43.24	245	11.89	0.04	54	473	28
23	23.6	60.5	270.74	40.21	370	10.45	0.18	48	478	19
24	29.5	61.7	355.61	32.65	290	16.32	0.07	54	660	25
25	23.5	55.8	322.79	31.35	287	11.04	0.03	50	456	28
26	22.5	54.7	250.62	33.65	370	12.76	0.12	61	476	26
27	23.6	44.7	261.78	32.67	400	10.45	0.16	34	821	43
28	29.4	58.4	276.85	23.65	468	9.43	0.04	38	448	50
29	43.48	41.13	280.54	27.43	280	10.45	0.02	43	650	51
30	42.45	40.32	278.54	23.54	460	12.03	0.03	41	720	40
31	40.21	50.35	300.45	30.78	380	9.32	0.12	40	459	39

S/N	C16:0	C18:1	BSFC (g/kWhr)	BTE (%)	EGT (^{0} C)	BMEP (bar)	CO (%)	Smoke intensity	NOx (ppm)	UHC (ppm)
32	39.43	55.43	285.05	32.76	380	10.45	0.21	42	700	52
33	42.56	50.45	260.45	22.09	410	15.23	0.07	60	710	48
34	37.16	46.93	290.54	35.05	420	9.05	0.04	57	651	27
35	35.76	50.43	315.85	35.87	410	10.45	0.12	43	552	40
36	40.42	49.32	250.45	34.53	358	10.25	0.08	38	460	48
37	43.56	42.46	260.48	22.87	330	11.35	0.15	28	570	28
38	35.32	50.32	270.41	28.54	450	11.21	0.21	40	592	28
39	38.43	39.45	301.45	27.91	510	10.35	0.05	50	702	34
40	45.21	55.32	310.65	32.56	350	9.25	0.13	61	810	28
41	42.75	45.55	317.23	38.21	420	12.25	0.17	52	830	54
42	34.52	42.59	260.54	28.45	470	10.27	0.13	58	750	43
43	53.7	22.8	270.4	23.54	400	11.45	0.12	42	453	40
44	52.9	22.2	230.2	30.43	398	12.43	0.089	45	650	52
45	51.83	24.13	332.4	26.54	453	9.43	0.012	51	542	43
46	53	23.3	280.4	32.54	498	8.56	0.032	54	732	51
47	22.19	48.2	276.1	32.65	453	10.43	0.22	52	487	43
48	53.3	25	321.3	34.67	487	11.76	0.21	52	505	56
49	13.31	50.76	324.8	40.32	421	11.43	0.045	48	476	34
50	55.53	23.26	265.3	28.43	487	10.21	0.27	51	432	45
51	52.5	24.8	234.5	32.54	462	10.43	0.047	47	480	48
52	54.1	22.6	301.2	29.56	487	10.04	0.012	41	440	47
53	48.9	23.18	261.4	33.06	442	11.25	0.05	51	455	51
54	73.73	16.93	230	39.54	398	11.54	0.081	60	475	48
55	66.02	20.43	265.1	33.65	436	10.56	0.127	53	432	53
56	69	23.87	223.5	35.91	429	12.15	0.034	56	624	46
57	67.7	20.5	230.03	39.23	387	12.23	0.068	45	654	32
58	63.29	23.68	267.3	33.09	492	10.45	0.014	51	562	27
59	77.89	32.78	243.1	37.43	431	12.56	0.043	49	467	54
60	63.5	24	276.3	37.89	342	12.54	0.015	46	480	34
61	42.8	40.5	254.3	31.65	380	13.21	0.06	41	431	43
62	42.6	40.5	265.3	39.02	371	11.54	0.08	61	657	30
63	42.7	40.9	342.1	32.94	278	10.41	0.043	57	567	36

S/N	C16:0	C18:1	BSFC (g/kWhr)	BTE (%)	EGT (^{0} C)	BMEP (bar)	CO (%)	Smoke intensity	NOx (ppm)	UHC (ppm)
64	44.81	39.99	287.3	43	263	11.54	0.023	52	680	25
65	43.32	40.57	276.3	40.43	381	9.43	0.143	52	623	20
66	40.2	43.3	344.9	32.65	301	12.54	0.043	58	560	27
67	47.9	37	312.4	31.54	297	11.27	0.078	56	467	30
68	43.9	39	265.1	33.89	385	12.54	0.17	59	651	24
69	39.5	43.2	253.87	32.76	402	11.48	0.042	37	605	40
70	23.3	42.4	265.32	24.5	458	10.21	0.054	31	458	42
71	25.2	48.9	276.21	28.54	320	11.24	0.027	45	620	35
72	23.1	45.8	265.32	23.87	430	12.38	0.04	53	680	43
73	23.9	43.9	299.3	31.5	341	10.34	0.014	48	461	47
74	24.34	42.23	300	31.65	374	10.5	0.043	54	680	41
75	20.1	55.2	267.3	24.65	403	13.78	0.052	61	520	56
76	28.7	57.4	297	35.78	415	10.54	0.05	54	670	43
77	11.67	57.51	312.34	33.87	407	10.68	0.14	48	550	40
78	28.33	57.51	243.43	35.05	372	9.98	0.065	35	535	41
79	20.6	52.5	260.45	23.55	350	12.21	0.18	30	555	32
80	22.9	54.2	265.43	28.94	448	11.12	0.27	38	610	28
81	11.38	48.28	300.2	27.54	471	10.58	0.052	47	700	43
82	11.4	48.3	312.45	33.56	378	10.76	0.076	60	750	26
83	11.2	45.5	317.43	39.84	425	11.35	0.17	54	652	44
84	10.4	47.1	276.4	29.4	446	10.46	0.173	51	690	32
85	23.6	44.2	265.43	34	400	10.57	0.045	49	475	24
86	25.5	47.1	235.53	37.98	389	12.89	0.072	40	705	32
87	24.49	38.32	321.54	28.54	476	10.54	0.045	45	530	38
88	20.6	64	287.43	32.04	473	10.43	0.043	59	710	43
89	22.3	64.1	280.11	33.41	450	11.28	0.28	61	480	25
90	22.3	64.4	250.12	34.14	470	11.54	0.32	57	503	36
91	20.6	61.6	231.07	35.8	405	12.05	0.076	61	470	43
92	20.6	61.5	308.05	28.98	465	10.21	0.32	53	443	56
93	46.36	32.38	278.5	34.65	450	11.56	0.045	52	472	45
94	69.07	18.97	298.32	30.55	475	10	0.048	48	485	51
95	43.08	40.55	254.43	34	420	11.35	0.064	52	605	60

S/N	C16:0	C18:1	BSFC (g/kWhr)	BTE (%)	EGT (^{0} C)	BMEP (bar)	CO (%)	Smoke intensity	NOx (ppm)	UHC (ppm)
96	23.88	45.25	228.57	38.45	400	12.58	0.023	60	621	42
97	55.72	40.23	278.43	31	435	11.43	0.182	54	710	38
98	32.14	47.23	254.65	36.41	420	12.56	0.132	47	540	54
99	26.03	45.43	234.61	38.5	385	11.67	0.126	48	462	32
100	21.28	63.12	276.54	32.81	490	11.68	0.023	55	440	26
101	23.1	63.2	234.54	37	441	10.43	0.043	45	445	55
102	20.43	61.9	234.78	40.33	398	18.45	0.05	46	465	43
103	10.12	79.4	200.54	31.56	379	12.5	0.06	47	367	56
104	24.32	62.05	220.56	40.34	337	11.65	0.056	35	761	34
105	15.05	75.32	340.54	24	248	10.03	0.132	37	658	37
106	34.54	50.3	300	51	271	11.32	0.231	41	456	54
107	35.65	50.5	267.05	40.05	375	10.76	0.16	42	571	39
108	23.67	58.23	340.54	36.02	271	13.28	0.17	40	665	28
109	26.76	46.55	342	38.87	300	10.43	0.034	55	456	34
110	30.65	53.3	256.54	33.13	362	11.32	0.172	42	467	53
111	27.54	58.43	270	33.76	389	9.47	0.166	48	749	48
112	34.32	46.5	256.43	30.19	465	11.78	0.074	41	450	65
113	20.43	46.3	278.54	28.78	300	9.68	0.023	50	630	31
114	26.43	57.84	260	24.67	487	13.43	0.056	44	726	27
115	54.32	26.89	310.65	30.56	381	15.32	0.183	54	471	41
116	46.32	34.54	290.5	33.81	345	18.01	0.124	60	704	28
117	20.56	60.33	267.54	26.5	389	16.55	0.23	46	723	44
118	43.65	34.59	284.65	33.89	400	13.65	0.124	59	456	47
119	32.65	50.05	312.54	33.71	421	11.45	0.043	44	443	34
120	25.21	52.65	260.67	37.2	430	9.67	0.012	51	506	49
121	42.39	34.56	239.05	24.54	327	10.32	0.043	39	561	28
122	41.65	50.05	289.12	29.55	437	10.43	0.312	45	604	38
123	44.54	45.5	310.32	28.57	505	11.59	0.043	50	673	43
124	32.89	44.65	309.65	33.65	355	10.54	0.23	48	782	26
125	27.35	56.43	278.09	35.18	430	9.26	0.176	51	774	41

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III. RESULTS AND DISCUSSION

We developed an ANN model to predict the engine performance and emission characteristics of an unmodified CI engine with C16:0 and C18:1 as inputs using the BP-LM algorithm. The predicted engine performance was BSFC, BMEP, BTE, and EGT, while four emission characteristics, namely CO, smoke intensity, UHC, and NOx were predicted. The two input parameters were palmitic and oleic acids. Figure 4 shows the structure of ANN consisting of input, hidden, and output layers and their respective number of nodes generated by the ANN model developed on a MATLAB R2017b NNTool. Data were sourced from literature for the training and validation of the model while the engine performance and emission characteristics of optimal FAME candidate produced by the transesterification of WPO and analyzed by GCMS were predicted by the trained ANN model. The overall correlation coefficient of the ANN model is shown in Fig. 5. The regression

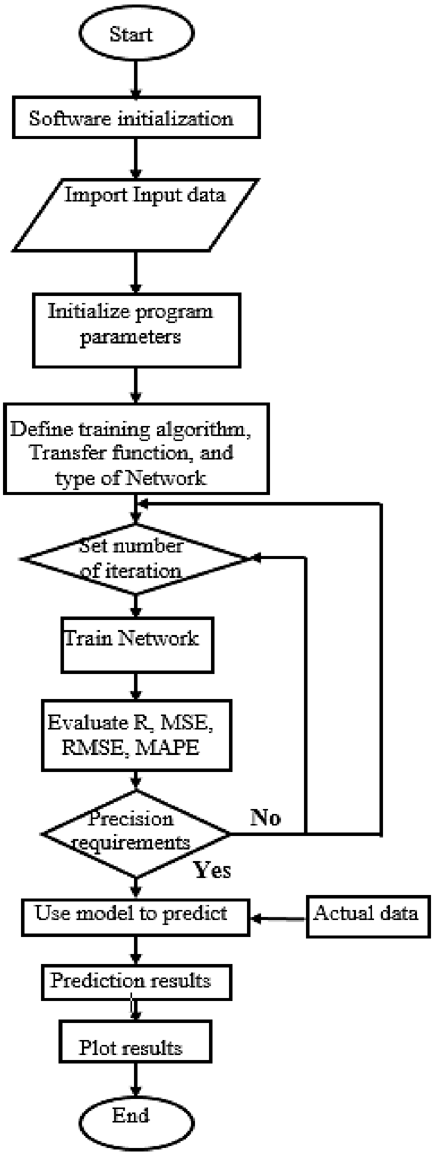

Fig. 3. Flow chart of ANN model

coefficient of the training, validation, and test data gave satisfactory value, an indication of high predictive proficiency of the established model. The outcome of the overall correlation coefficient for the present model is an improvement on the outcome of similar efforts [58-60].

The performance indices of the trained ANN model using regression and other statistical error parameters as well as comparison of the predicted data with experimental data for 15 different test cases are presented in Fig. 5–14. The prediction of output parameters yielded impressive outcomes for BSFC, BMEP, BTE, CO, EGT, UHC, NOx, and smoke intensity with commendable and reliable values of R, MSE, RMSE, and MAPE for each parameter. This indicates the accuracy, sensitivity, capacity, and capability of the developed model to simultaneously predict important engine performance and emission parameters that can be relied upon.

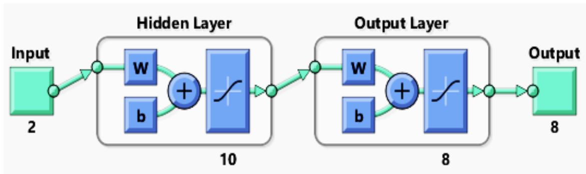

Fig. 4. Neural network model created using NNTool box [44]

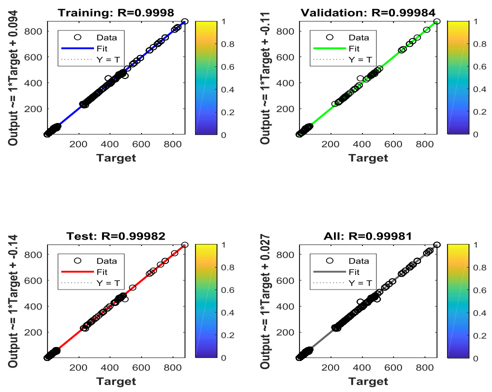

Fig. 5. The overall correlation coefficient of the ANN model.

Figure 6a compares the ANN predicted data with the experimentally measured data. With R-value of 0.9984, MSE, RMSE, and MAPE values of 0.009906, 0.09953 g/kWh, and 1.729 % respectively, the model performed acceptably. The model was also applied to predict the BSFC of some FAME samples. This result is comparable to the correlation coefficient of 0.9968, and MSE of 0.0177 reported by Syed et al. [61]. The outcome, as shown in Fig. 6b, was commendable and can be relied upon to arrive at a sound decision on the fuel. Bearing in mind the importance of BSFC as an engine performance parameter, and the relationship between fuel consumption, power output and efficiency of an oxygenated fuel like FAME, this model will be useful to determine the behavior of FAME from its palmitic and oleic acid concentrations. Figures 7a and 7b illustrate

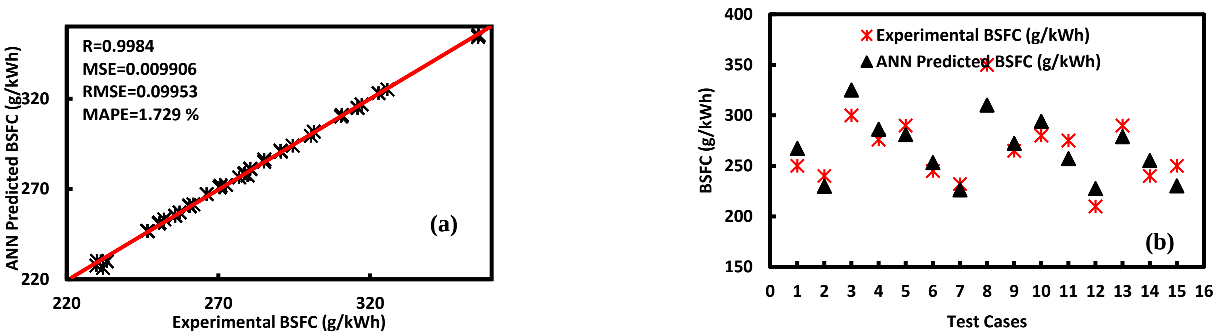

Fig. 6. (a) Regression plot for BSFC (b) Comparison of experimental and ANN predicted BSFC

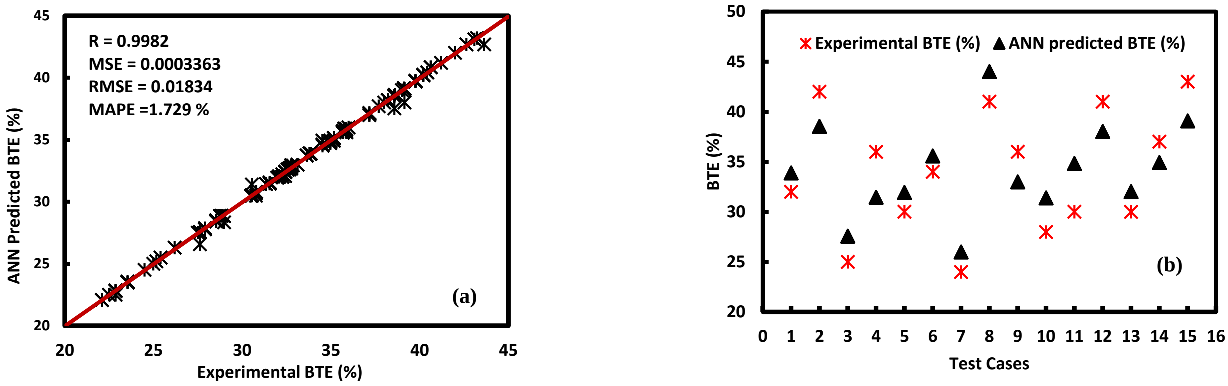

Fig. 7. (a) Regression plot for BTE (b) Comparison of experimental and ANN predicted BTE

the ANN predicted BTE versus experimental BTE and the outcome of the predicted data for 15 experimental test cases. With R of 0.9982, MSE of 0.0003363, RMSE of 0.09953 % and MAPE of 1.729 %, the developed ANN model was satisfactory and acceptable. These results were comparable with the outcome of similar investigations reported in the literature [59, 62].

The correlation coefficient and other statistical errors of the developed ANN model for BMEP were found to be within acceptable levels throughout the investigation despite the nonlinear relationship between BMEP and the FA composition of biodiesel. As shown in Fig. 8a and 8b, the model provided a satisfactory outcome with statistical errors within acceptable limits. The R-value of 0.9991, MSE value of 0.001032, RMSE value of 0.03212 bar and MAPE value of 2.674 % showed good predictive capabilities of the model. Figure 9a and 9b show the relationship between the experimental and ANN predicted data of EGT. The performance index of the model indicates an R of 0.999 and RMSE of 0.03212. This result is comparable with the R-values of 0.9995 reported by Syed et al. [61] and 0.99754 reported by Javed et al. [28].

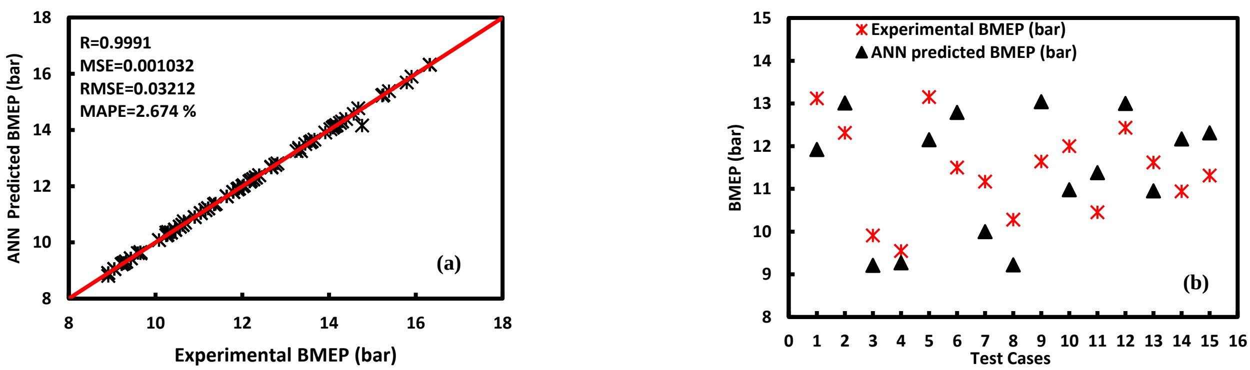

Fig. 8 (a) Regression plot for BMEP (b) Comparison of experimental and ANN predicted BMEP

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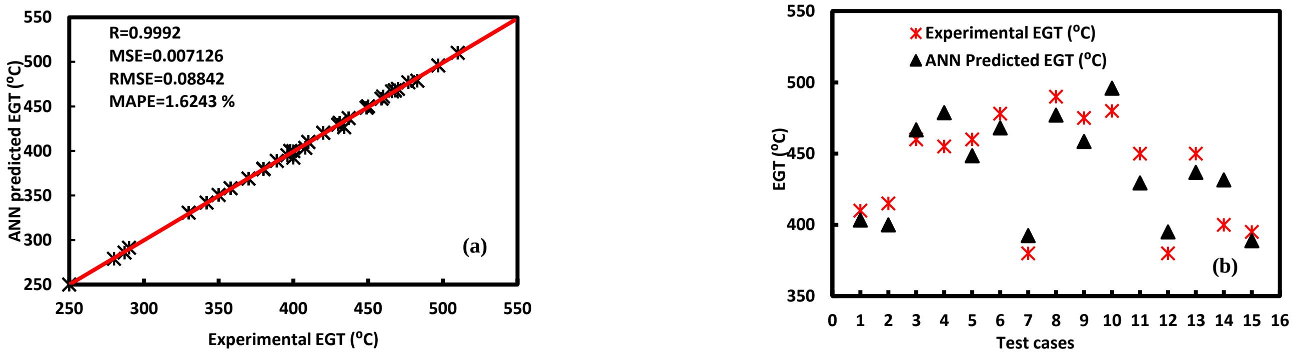

Fig. 9. (a) Regression plot for EGT (b) Comparison of experimental and ANN predicted EGT

The developed model predicted CO and NOx within acceptable limits. The predicted CO and NOx were close to the experimentally measured values. This is shown by the R-value near 1. The value of MSE, RMSE, and MAPE show the high prediction accuracy of the model. As shown in Fig. 10a and b, and 11a and b the gap between the experimentally determined and ANN predicted values are negligible for CO and NOx emissions. Due to the effects of CO emission on humans and the environment the parameters need to be accurately predicted so as to be able to drastically reduce CO emissions. High emissions of NOx in a CI engine remains one of the drawbacks for the application of FAME as a CI engine fuel. Researchers are still working on lowering the NOx emission in line with standards. This model accurately predicts the emissions of CO and NOx gases thereby making real-time engine tests unnecessary. This result is an improvement on the outcome of similar studies available in the literature [62, 63].

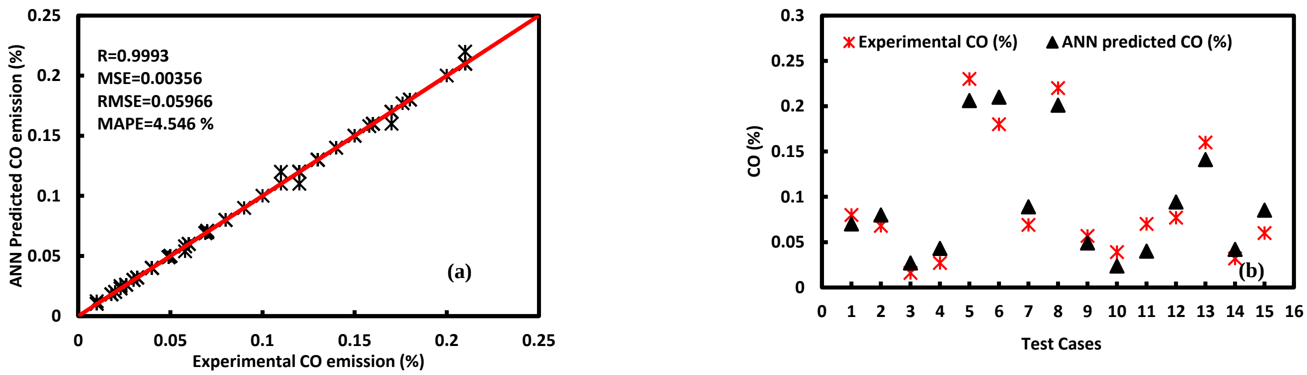

Fig. 10. (a) Regression plot for CO (b) Comparison of experimental and ANN predicted CO

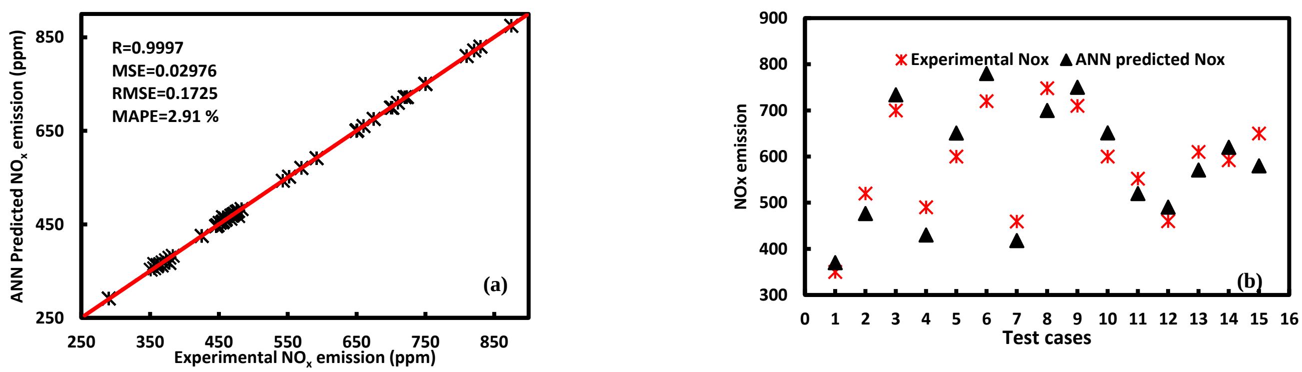

Fig. 11. (a) Regression plot for NOx (b) Comparison of experimental and ANN predicted NOx

It can be deduced from the outcomes of the model prediction that the ANN predicted values agree well with the experimentally measured values. This reveals that the developed ANN model has satisfactorily determined the UHC and smoke intensity of CI engine fueled with FAME. The R-value was found to be 0.9995 and 0.9966 for UHC and smoke intensity, respectively. The closeness of these R values to 1 signifies the high accuracy of the prediction. For the UHC emissions the RMSE value is 0.1135 and MAPE value is 2.503 % (Fig. 12a and 12b) and for the smoke intensity the RMSE is 0.02154 and the MAPE is 2.294 % (Figure 13a and 13b). These small RMSE and MAPE values are indicative of the high accuracy of the developed model [41, 61, 63].

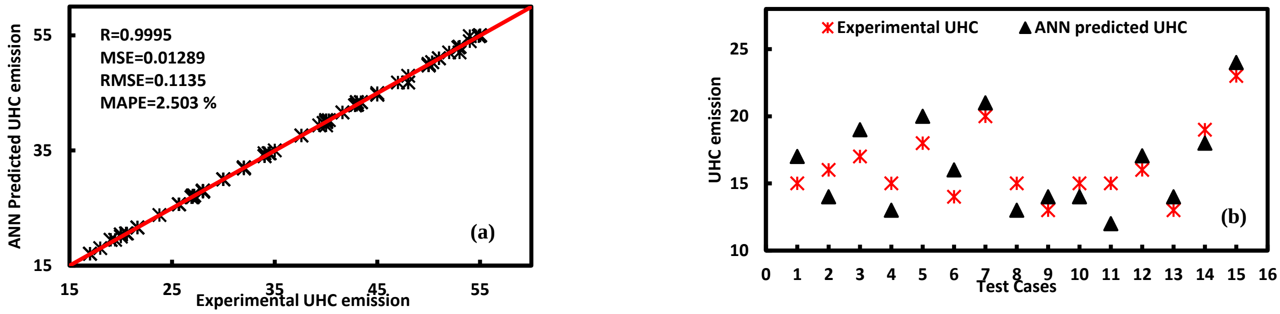

Fig. 12. (a) Regression plot for UHC (b) Comparison of experimental and ANN predicted UHC

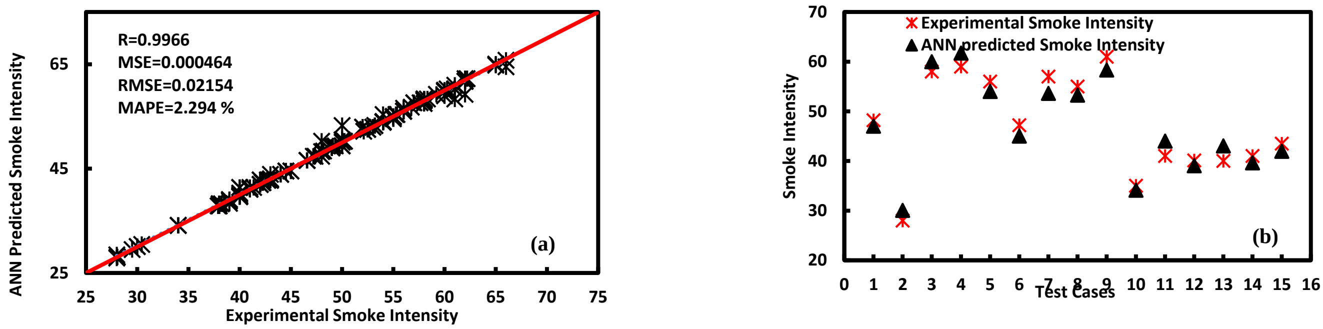

Fig. 13. (a) Regression plot for Smoke intensity (b) Comparison of experimental and ANN predicted Smoke intensity

III.I. Prediction of Engine Performance and Emissions of Optimal FAME

A well-trained ANN model was deployed to predict the BSFC, BMEP, BTE, CO, EGT, UHC, NOx, and smoke intensity of CI engine fueled with the optimal FAME candidate produced to certain configurations. The two most important FA composition identified were C16:0 and C18:1 and these were used as inputs. The outcomes of the ANN predictions were compared with the outcomes of real-time CI engine tests from the literature as shown in Table 3. In terms of engine performance, the optimal candidates delivered encouraging performance parameters when compared with similar research outcomes. The BSFC was lower whereas the BTE was relatively high but at a lower EGT. The CO, NOx, UHC and smoke opacity emissions were found to be lower than all the outcomes of comparable investigations. The oxygenated fingerprint of the FAME candidate ensured better combustion which was reflected in the low CO emission. The low EGT also resulted in the low NOx emissions. These outcomes show that the computed optimal FAME candidates yielded better engine performance and emitted less regulated gases, thereby meeting the objective of developing a new fuel.

Table 3. Datasets for the ANN model

Parameter	unit	Present research	Arunkumar et al. [64]	Sanli et al. [65]	Subramaniam et al. [66]	Singh et al. [67]
BSFC	g/kWh	205	750	230 to 247	400 to 460	300 to 500
BTE	%	30	28	-	24 to 26	0 to 30
BMEP	bar	45	-	38 to 42	-	-
EGT	^{0} C	260	300	-	-	150 to 380
CO	%	0.05	0.07	700 to 6000(ppm)	-	0.05 to 0.09
NOx	ppm	400	470	1400 to 1550	300 to 900	350 to 980
UHC	ppm	18	35	22 to 26	-	70 to 110
Smoke intensity	-	50	55	-	72 to 102	9 to 50

III.I. Prediction of Engine Performance and Emissions of Optimal FAME

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IV. CONCLUSION

In this study ANN was developed and trained using secondary data mined from literature for the simulation and prediction of engine performance and emission characteristics. The validated model was used to predict the engine performance and emission of a computed optimal FAME mix. The MATLAB ANN model based on BP-LM algorithms with tangent-sigmoid transfer function was developed to predict engine performance and emission parameters of an unmodified CI engine fueled with FAME. We employed two input layers, one hidden layer with ten neutrons, and eight output layers using NNTool techniques to determine the BSFC, BMEP, BTE, CO, EGT, UHC, NOx, and smoke intensity.

The outcomes of the developed ANN model were evaluated using regression coefficient and other statistical error platforms as well as other performance metrics to compare the experimental data with ANN predicted data. A total of 749 data were mined from literature and used to train the model while the FA composition of the optimal FAME candidates were produced through the transesterification of WPO. Going by the results, the model performed very well with the experimental data matching the ANN predicted data with an overall regression coefficient (R) of 0.9998. For the engine performance parameters, R varied between 0.9982 and 0.9991 while the RMSE and MAPE ranged between 0.01834 and 0.09953, and 1.729 % and 2.674 % respectively. The R, RMSE, and MAPE for the emission parameters varied from 0.9966 to 0.9997, 0.02154 to 0.1725, and 1.6443 % to 4.546 % respectively.

From the foregoing, the optimal FAME candidates, namely, C16:0 with results of 36.4 % and C18:1 with 59.8 % demonstrated better engine performance and mitigated emission characteristics. The developed model accurately and reliably predicted the performance and emission parameters within acceptable limits. Thus, these two FAs are sufficient to accurately predict the engine performance and emission characteristics of a conventional and unmodified CI engine. Thus, FAME with concentrations of C16:0 and C18:1 can be trusted to perform optimally and generate mitigated emissions. It is thus safe to conclude that the developed ANN model has been able to reliably and conveniently imitate real engine performance and emission characteristics within satisfactory prediction accuracy and efficiency.

Going forward, this narrative should be stretched further to include the use of FA compositions of various feedstocks to predict, within reasonable accuracy, combustion, fuel mixing, and heat release rate with a view to evaluating their influence on engine performance, combustion, and emission characteristics of an unmodified CI engine.

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