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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

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 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].

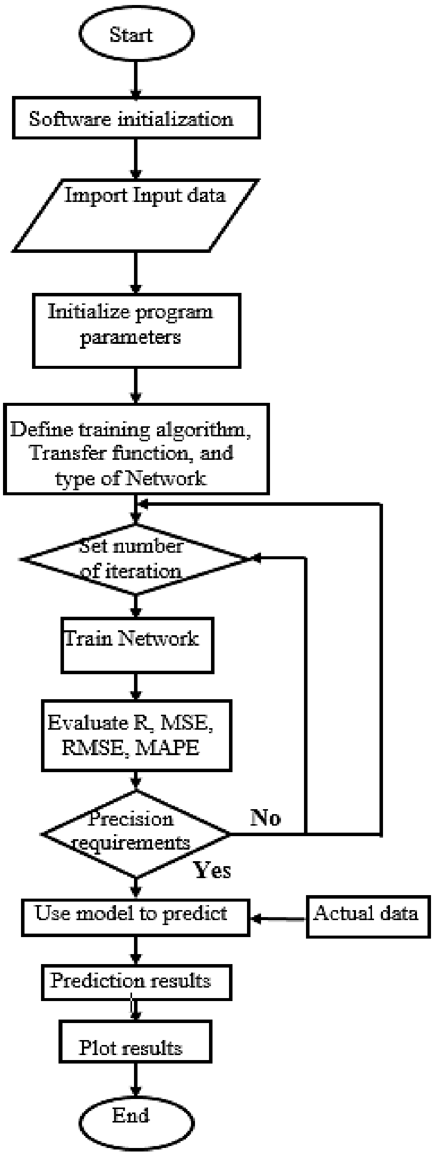

Fig. 3. Flow chart of ANN model

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.

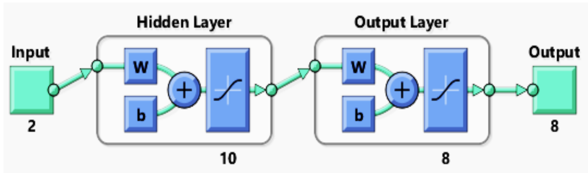

Fig. 4. Neural network model created using NNTool box [44]

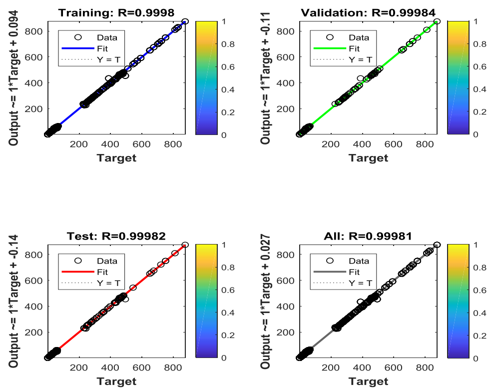

Fig. 5. The overall correlation coefficient of the ANN model.

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

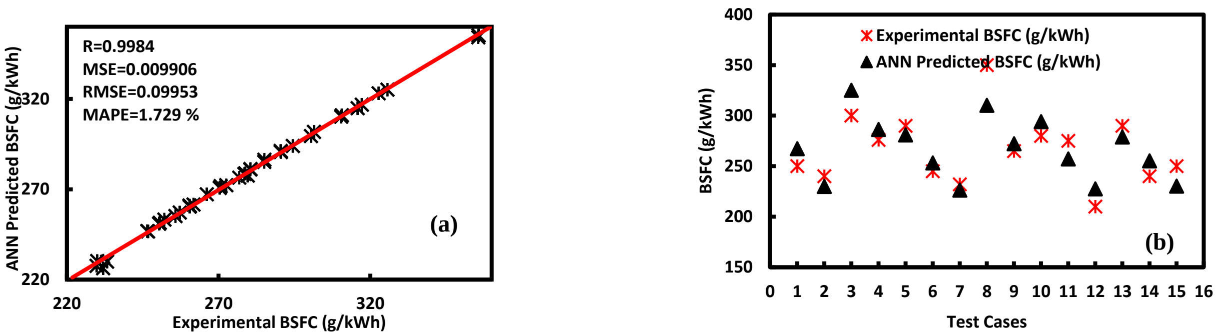

Fig. 6. (a) Regression plot for BSFC (b) Comparison of experimental and ANN predicted BSFC

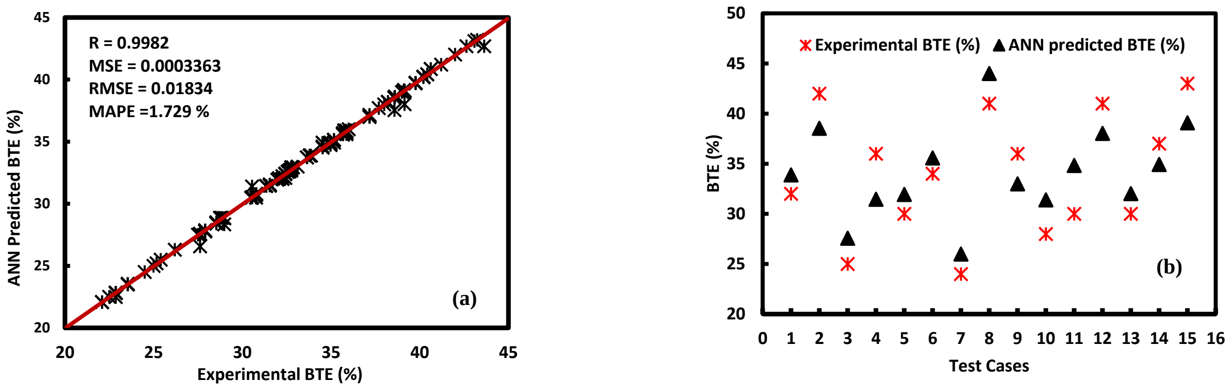

Fig. 7. (a) Regression plot for BTE (b) Comparison of experimental and ANN predicted BTE

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].

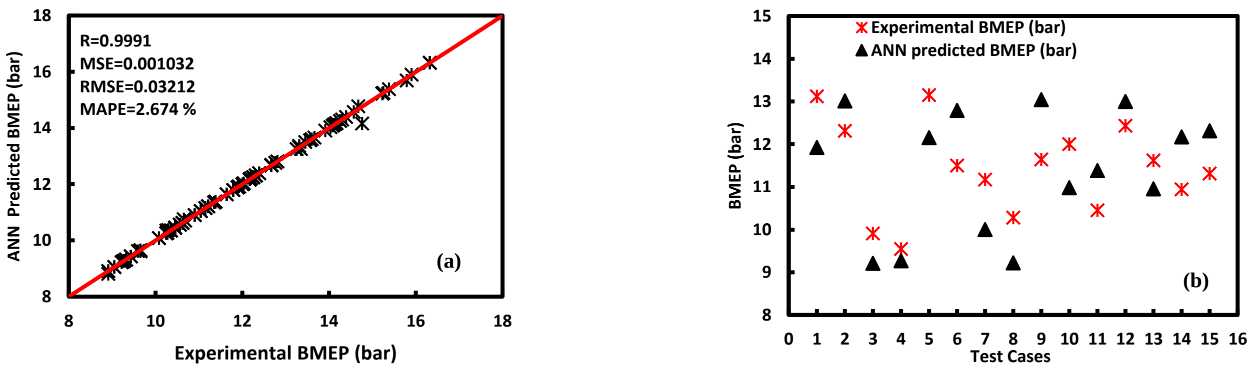

Fig. 8 (a) Regression plot for BMEP (b) Comparison of experimental and ANN predicted BMEP

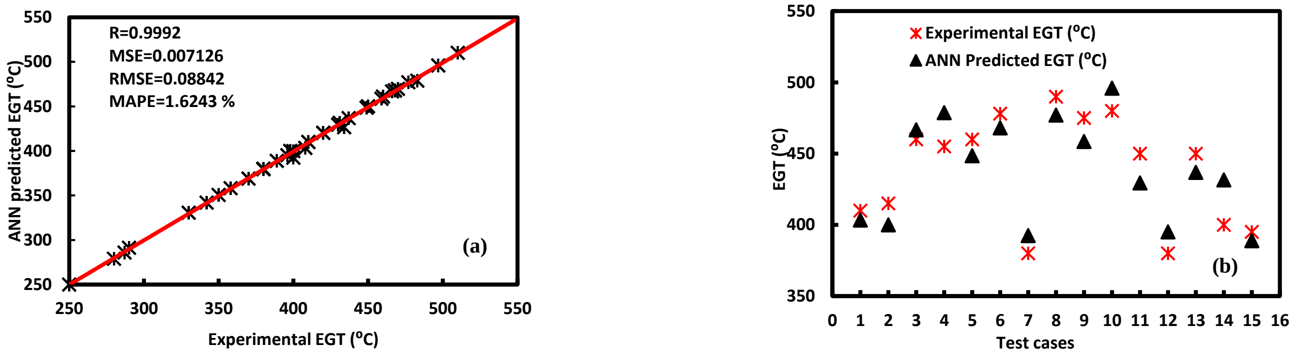

Fig. 9. (a) Regression plot for EGT (b) Comparison of experimental and ANN predicted EGT

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].

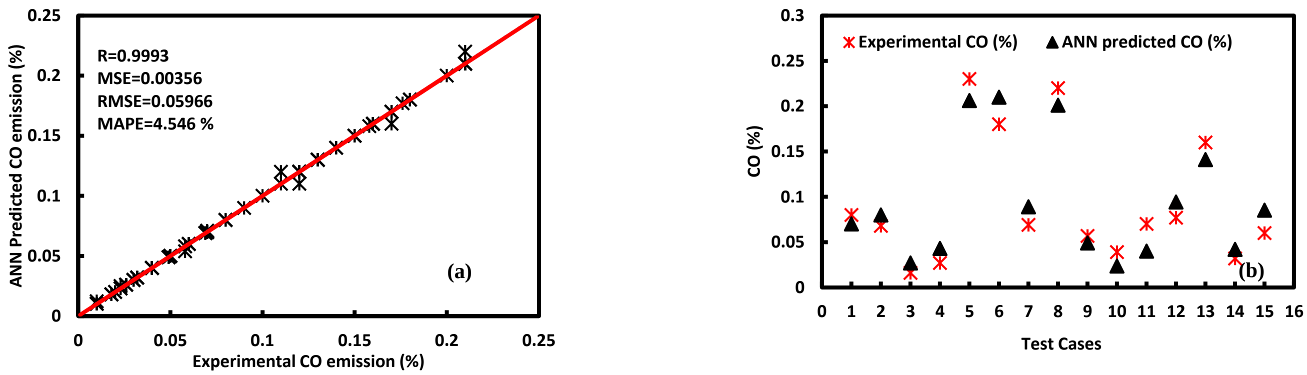

Fig. 10. (a) Regression plot for CO (b) Comparison of experimental and ANN predicted CO

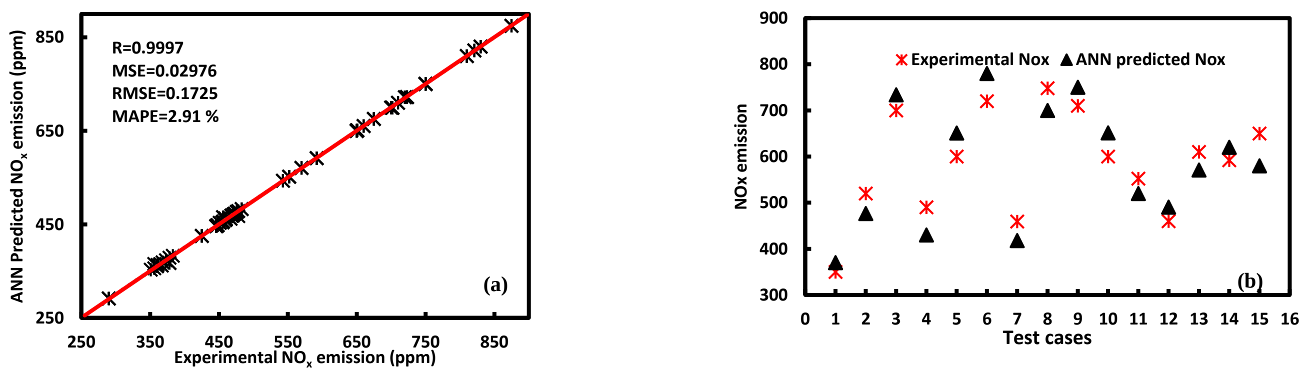

Fig. 11. (a) Regression plot for NOx (b) Comparison of experimental and ANN predicted NOx

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].

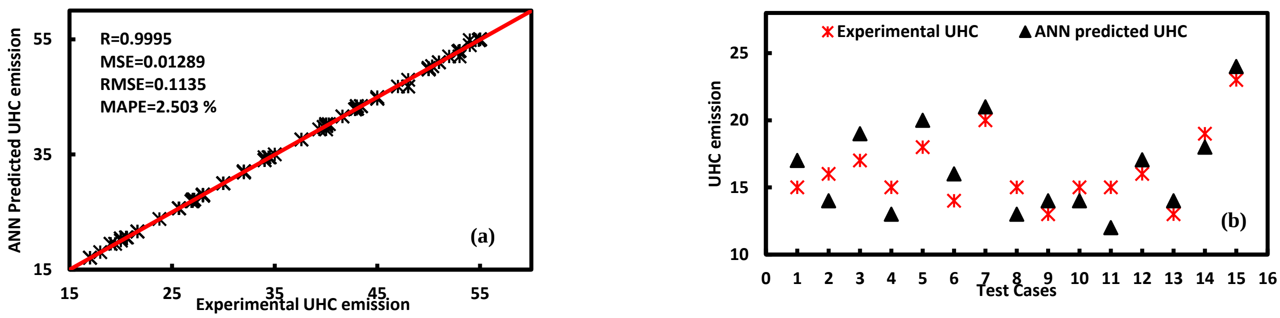

Fig. 12. (a) Regression plot for UHC (b) Comparison of experimental and ANN predicted UHC

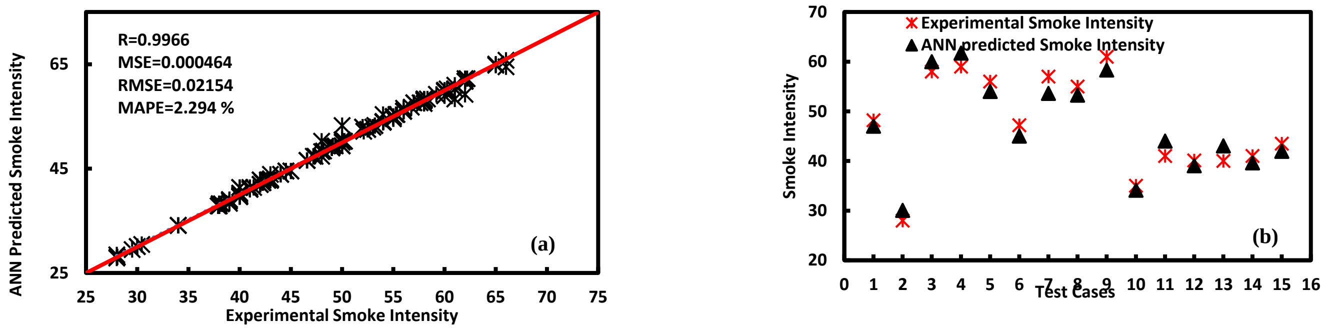

Fig. 13. (a) Regression plot for Smoke intensity (b) Comparison of experimental and ANN predicted Smoke intensity

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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