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Original Article

Modelling of multiple biodiesel-emitted nitrogen oxides using ANN approach

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ABSTRACT

This research paper focuses on modelling of nitrogen oxides emitted by diesel engine for multiple biodiesel blends. A lot of research work has observed that the properties of biodiesel blends affect the nitrogen oxide emissions. To this aim, total of fifteen blends of multiple biodiesels are prepared on vol. % by using four non-edible category biodiesels. The suitability and quality of the biodiesel and diesel blends are tested through a characterization and found within the permissible limits of ASTM. The experimentation has been carried out on a direct injection compression ignition (DICI) engine with constant speed and varying loading condition from no load to full load in a step of 25%. During the experimentation, the NOx emissions are measured using a Netel MGA-2 exhaust gas analyzer. The study revealed that several properties such as viscosity, density, mean gas temperature, etc. affect NOx emission. In addition, NOx emission increases with an increase in BPs. The artificial neural network (ANN) is performed by considering physicochemical and thermal properties as a function. The ANN predicts the estimated NOx with an accuracy of 0.99.

1. Introduction

Several types of pollutants emit from the engine emissions after burning of the fuels which are harmful to human beings in general and climates in particular [1]. Incomplete combustion of an engine results in the release of harmful pollutants such as carbon monoxide (CO), hydrocarbons (HC), and particulate matter (PM) emissions [2–4]. Flavorless, odorless, and colorless most noxious matter found in exhaust emissions known as carbon monoxide (CO). If the molecules are not oxidized then hydrocarbons releases from the combustion process as a byproduct whereas carbon atoms are not burned due to limited oxygen availability leads to produced carbon monoxide and both the terms hydrocarbons and carbon monoxides have adverse effect on human health [5]. The carbon dioxide emissions are linked to fuel consumptions, more the fuel consumption which leads to increases the carbon dioxide emissions. The pollutant levels basically dependent on the maintenance condition of the vehicle and vehicle technology. Exhaust emission pollutants also affected by different aspects such as style of driving, vehicle condition, ambient temperatures [6]. The various emission parameters of vehicle engines are measured by exhaust gas analyzer and described in vol. % and ppm format. The light-duty and passenger vehicles require emission levels in g/km whereas heavy-duty vehicle prefers in g/kWh when the comparison required with European vehicle emission standards [7,8]. The interconnection between emission parameters of vehicles and specific fuel consumptions (SFCs) are observed in open literature [9–11].

1.1. Nox emission formation mechanism

NOx can be formed by five different ways. Prompt NOx is also known as Fenimore mechanism. Especially it is formed at the front of the flame when enriched air–fuel mixture with absence of oxygen. In oxidation the radicals of CH with molecular nitrogen (N_2) lead to form cyan hydric acids (HCN) and oxides of nitrogen (NO). Generally amines or cyano compounds conveyed and rehabilitated to intermediate compounds to

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Nomenclature

Abbreviations	Full-form
CN	Cetane Number (No.)
D	Diesel, (B0)
Exp. and Est.	Experimental and Estimated
F	Flash point (deg.C)
HV	Heating Value (MJ/kg)
JB (JOME)	Jatropha biodiesel (Jatropha oil methyl ester)
KB (KOME)	Karanja Biodiesel (Karanja oil methyl ester)
MB (MOME)	Mahua Biodiesel (Mahua oil methyl ester)
NB (NOME)	Neem Biodiesel (Neem oil methyl ester)
ν	Kinematic viscosity (mm^2/s)
ρ	Density (kg/m^3)

form NO when radicals of hydrocarbons react molecular nitrogen (N_2) [12]. Zeldovich mechanism that would leads to intermediate route in lean fuels having equivalence ratio (φ) < 0.8 under low temperatures. The thermal NOx formation depends on the zone temperature, air–fuel ratio, oxygen concentration and equivalence ratio and last but the most important reaction time [13]. Table 1 provides the comparative literature review of NOx emission and their variations for different biodiesel-diesel blends under different operating conditions.

Due to popularity of numerical investigations in the presence scenario various techniques such as multiple objective optimization [22], biodiesel production [23,24], production using RSM [25], production using catalyst (CaO) [26,27], ternary blends [28] intelligent ANN-RSM [29], dual-fuel engine [30], Taguchi L_{16} orthogonal array [31], and optimal blending ratio [32]. Ramadhas et al. applied multi-layer feed forward neural network for predicting the cetane number using fatty acid compositions of biodiesel and predicted the values of CN using ANN. They have compared the experimental values with numerical and found that the predicted values are in agreement with experimental

Table 1
Variation of NOx for different biodiesel-diesel blends.

Blends Utilized	Test set-up	Testing conditions	NOx emissions		References
			Trend	Variations from neat diesel (%)	
Neat JOME	Four cylinder, turbocharged, intercooled	RPM 2000 with varying BMEP	↑	13.9	[14]
JOME, B5	Four cylinder, turbocharged, intercooled	RPM 2000 with varying BMEP	↑	1.02	[14]
JOME, B10	Four cylinder, turbocharged, intercooled	RPM 2000 with varying BMEP	↑	2.06	[14]
JOME, B10	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	1.61	[15]
JOME, B20	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	5.46	[15]
JOME, B20	Mitsubishi Pajero 4D56T engine	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	14.22	[16]
JOME, B20	Four cylinder, turbocharged, intercooled	RPM 2000 with varying BMEP	↑	4.74	[14]
JOME, B50	Four cylinder, turbocharged, intercooled	RPM 2000 with varying BMEP	↑	5.71	[14]
Neat POME	Yanmar L48N engine	RPM ranges 1800–3000	↑	8.60	[17]
POME, B10	Yanmar TF 120M, single cylinder, Naturally aspirated, water cooled	RPM ranges 1000–2400 rpm with full throttle condition	↑	4.81	[15]
POME, B10	Four cylinder, water cooled	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	16.0	[18]
POME, B10	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	4.79	[19]
POME, B20	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	7.91	[19]
POME, B20	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	8.03	[15]
POME, B20	Mitsubishi Pajero 4D56T engine	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	6.91	[16]
POME, B30	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	10.72	[19]
5% JOME + 5% POME + 90% diesel	Greaves Cotton Ltd. Engine	BP ranges 0.5–2.5 kW	↑	5.3	[20]
10% JOME + 10% POME + 80% diesel	Greaves Cotton Ltd. Engine	BP ranges 0.5–2.5 kW	↑	9.2	[20]
50% JOME + 50% POME	Yanmar TF 120M engine	RPM ranges 1000–2400 rpm with full throttle condition	↑	28.0	[19]
80*% POME + 20% methyl oleate (MO)	Yanmar L48N engine	RPM ranges 1800–3000	↑	10.60	[17]
70% POME + 30% MO	Yanmar L48N engine	RPM ranges 1800–3000	↑	12.61	[17]
60% POME + 40% MO	Yanmar L48N engine	RPM ranges 1800–3000	↑	13.50	[17]
50% POME + 50% MO	Yanmar L48N engine	RPM ranges 1800–3000	↑	14.90	[17]
MOME, B10	Four cylinder, water cooled	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	13.0	[18]
MOME, B20	Mitsubishi Pajero 4D56T engine	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	18.56	[16]
KOME, B10	Four cylinder, water cooled	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	9.0	[18]
KOME, B20	Four cylinder, water cooled	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	12.0	[18]
NOME, B10	Kirloskar single cylinder, water cooled	RPM 1500 rpm with BP ranges from 0.5 to 3.5 kW	↓	21.875	[21]

(*continued on next page*)

Table 1 (*continued*)

Blends Utilized	Test set-up	Testing conditions	NOx emissions		References
			Trend	Variations from neat diesel (%)	
NOME, B20	Kirloskar single cylinder, water cooled	RPM 1500 rpm with BP ranges from 0.5 to 3.5 kW	↓	8.375	[21]
NOME, B20	Naturally aspirated, air cooled	Load variations ranges within 0–1	↑	67.29	[21]
NOME, B30	Kirloskar single cylinder, water cooled	RPM 1500 rpm with BP ranges from 0.5 to 3.5 kW	↓	18.875	[21]
5% KOME + 5% MOME + 90% diesel	Four cylinder, water cooled	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	14.0	[18]
10% KOME + 10% MOME + 80% diesel	Four cylinder, water cooled	RPM ranges 1000–4000 in a step of 500 rpm with full throttle condition	↑	17	[18]

Table 2
Multiple biodiesel-diesel with their % contribution in preparation of blends.

Blend No.	Blend Name	Contribution of multiple biodiesel-diesel in vol. %				
		Diesel (D)	Jatropha (J)	Karanja (K)	Mahua (M)	Neem (N)
1	Neat Diesel (B0)	100	–	–	–	–
2	D90JK10	90	5	5	–	–
3	D90JM10	90	5	–	5	–
4	D90JN10	90	5	–	–	5
5	D90KM10	90	–	5	5	–
6	D90KN10	90	–	5	–	5
7	D90MN10	90	–	–	5	5
8	D90JKMN10	90	2.5	2.5	2.5	2.5
9	D80JK20	80	10	10	–	–
10	D80JM20	80	10	–	10	–
11	D80JN20	80	10	–	–	10
12	D80KM20	80	–	10	10	–
13	D80KN20	80	–	10	–	10
14	D80MN20	80	–	–	10	10
15	D80JKMN20	80	5	5	5	5

Table 3
Characterization of physicochemical and thermal properties.

Blend No.	(ρ)	(ν)	(F)	(CN)	(HV)
	kg/m^3	mm^2/s	°C	No.	MJ/kg
1	830	2.50	52	51.15	42.180
2	833	2.71	59	44.35	41.720
3	832	2.74	56	44.75	41.830
4	834	2.65	58	43.83	41.590
5	833	2.79	57	44.15	41.670
6	835	2.75	61	43.23	41.430
7	833	2.77	56	44.14	41.670
8	834	2.77	57	43.61	41.529
9	836	2.97	67	42.58	41.257
10	836	3.06	63	42.29	41.180
11	837	2.92	66	42.05	41.116
12	836	3.27	65	42.06	41.120
13	838	3.17	69	41.24	40.902
14	838	3.18	64	41.02	40.846
15	837	3.13	65	41.70	41.025
Biodiesel limits as per ASTM D-6751	–	1.9–6.0	52 min	40 min	–
Diesel limits as per ASTM D-975	–	1.3–4.1	130 min	47 min	–
Uncertainty in %	1.50	1.00	1.00	1.00	1.75

values [33]. Similar work is conducted by Jatinder Kumar et al. for evaluating of physicochemical properties of various mixtures of biodiesel and diesel. They have applied three different ANN algorithms i.e. batch gradient, descent with momentum, Levenberg-Marquardt and scaled conjugate gradient and compared the values with experimental. They found that LM algorithm gave better results compared to other algorithms [34]. Bhatt and Shrivasatava [35] conducted literature review on the application of ANN for predicting the performance of IC engine. Ghobadian et al. applied ANN modeling for predicting the performance and emission characteristics of CI engine fuelled with waste cocking biodiesel using multi-layer perception network model (MLP). The values of HC emissions are predicted with an accuracy R = 0.999 [36]. Similar model is applied by Hidayet Oguz et al. [37] for predicting the performance of CI engine fuelled bioethanol blends with the accuracy of R = 0.9994. Authors also performed experimentation by using different alcohol blends with biodiesel and studied how alcohol enhance the performance. Combustion and emission characteristics [38]. From the literature review it was found that many properties of biodiesel and diesel need to be considered because of their impacts on engine performance and emission characteristics. The NOx emission play an important role in the diesel engine emission category and it is affected by several physicochemical and thermal properties of the biodiesels. To this aim, the present research work focuses on the physicochemical and thermal properties of the multiple biodiesel blends at the preliminary level. Further experimentation has been extended for the evaluation of emission characteristics of DICI engine using blends under consideration. The modelling on nitrogen oxides emission has been performed by using artificial neural network (ANN) and results of experimentation and estimated (through ANN) are compared.

2. Experimental program

2.1. Blends preparation and characterization

Biodiesels from second generation category are utilized on vol. % in preparation of multiple biodiesel-diesel blends. Multiple biodiesels and their combinations based on seasonal availability and physicochemical and thermal properties are closer to the neat diesel [39]. Total fifteen blends including neat diesel are prepared by using four different biodiesels [39,40]. Each biodiesel is having constant vol. % proportion in the blends category of dual and multiple biodiesel-diesel. The detail

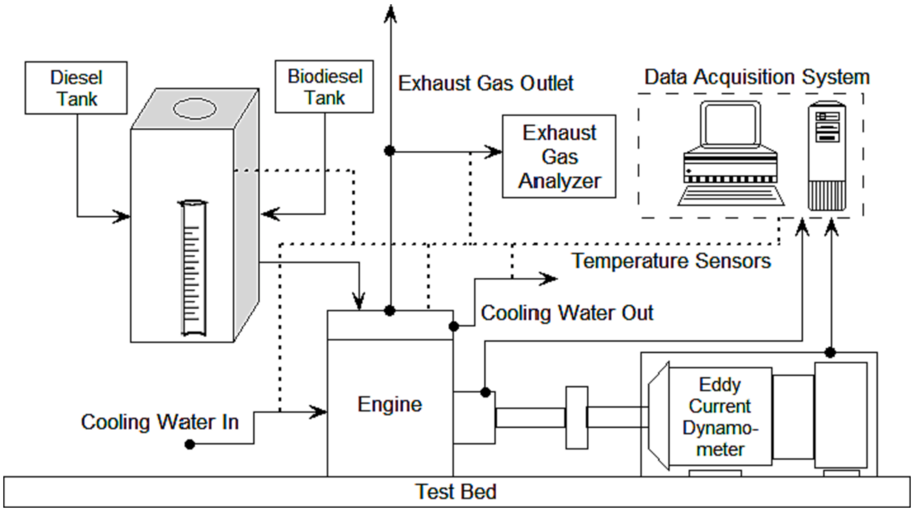

Fig. 1. Engine test-rig.

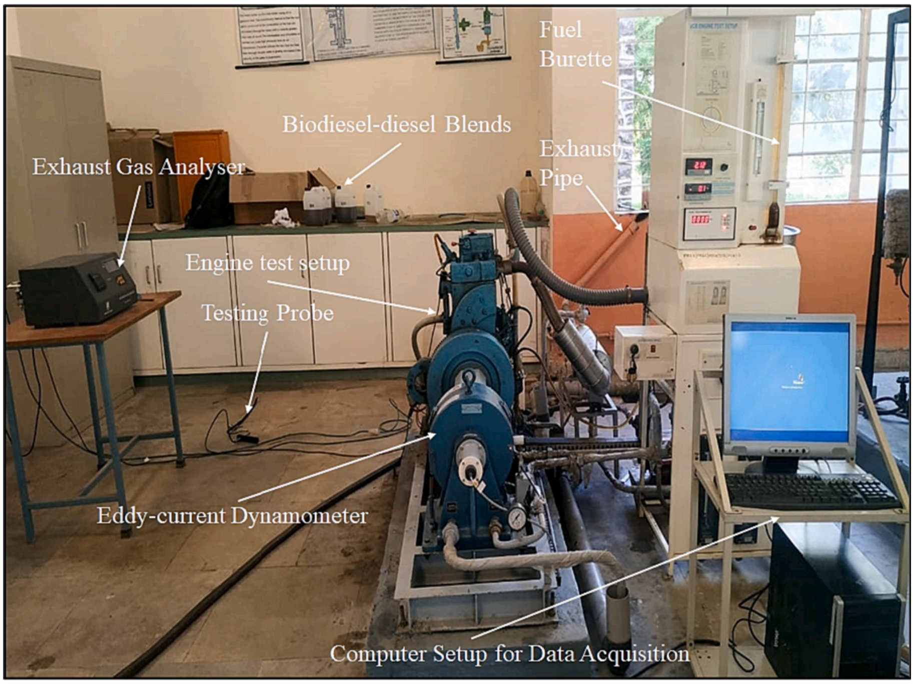

Fig. 2. Real Photograph of Engine test-rig.

Table 4
Technical Specification of DICI engine Test-rig.

Particulars	Specifications
Manufacturer	Kirloskar make TV-1
Aspiration Type	Naturally-aspirated
Injection Type	Direct Injection (DI)
No. of Cylinder	1
No. of stroke	4
Bore × stroke (mm)	80 × 110
Displacement (cc)	661
Compression ratio (CR)	17.5
Rated power (kW)	5.2 kW
Engine Speed	1500 rpm
Type of cooling	Water-cooled
Dynamometer Type	Eddy current
Dynamometer rating	7.2 kW

nomenclature of multiple biodiesel-diesel blends are given in Table 2.

The suitability and quality of the biodiesel tested at the preliminary level through characterizations. The physicochemical and thermal properties are tested as per the ASTM standards. The heating value (HV), kinematic viscosity (ν), flash point (F), density (ρ), and cetane number (CN) are measured as per the ASTM standards of D-240, D-445, D-93, D-941, and D-613. Table 3 provides the physicochemical and thermal properties characterization.

2.2. Experimental analysis

The experimental analysis has been performed on stationary diesel engine test-rig. The experimentation has been performed by using full constant speed of 1500 at variable loading from 0 to 100%. Total five loading conditions and the data pertaining to performance characteristics such as rpm, temperatures, specific fuel consumption (SFC), etc. have been recorded through the data acquisition system of the engine

Table 5
Technical specifications and resolution of exhaust gas analyser.

Particulars	Measurement Technique	Measurement Range	Resolution	Accuracy (Abs.)	Accuracy (Rel.)
Make	Netel	–	–	–	–
Model No.	MGA-2	–	–	–	–
Operating system	Micro-controller driven				
CO	NDIR	0–9.99 vol%	0.01%	±0.03%	±3%
CO_2	NDIR	0–20 vol%	0.10%	±0.04%	±4%
HC	NDIR	0–20000 ppm	1 ppm	10 ppm	±5%
O_2	NDIR	0–25 vol%	0.01%	±0.1%	±3%
NOx	Electrochemical	0–5000 ppm	1 ppm	25 ppm	±5%

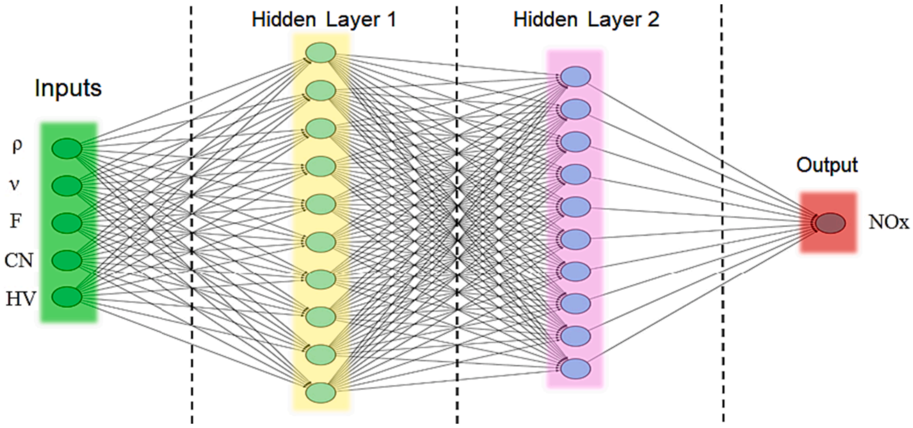

Fig. 3. Architecture of ANN model.

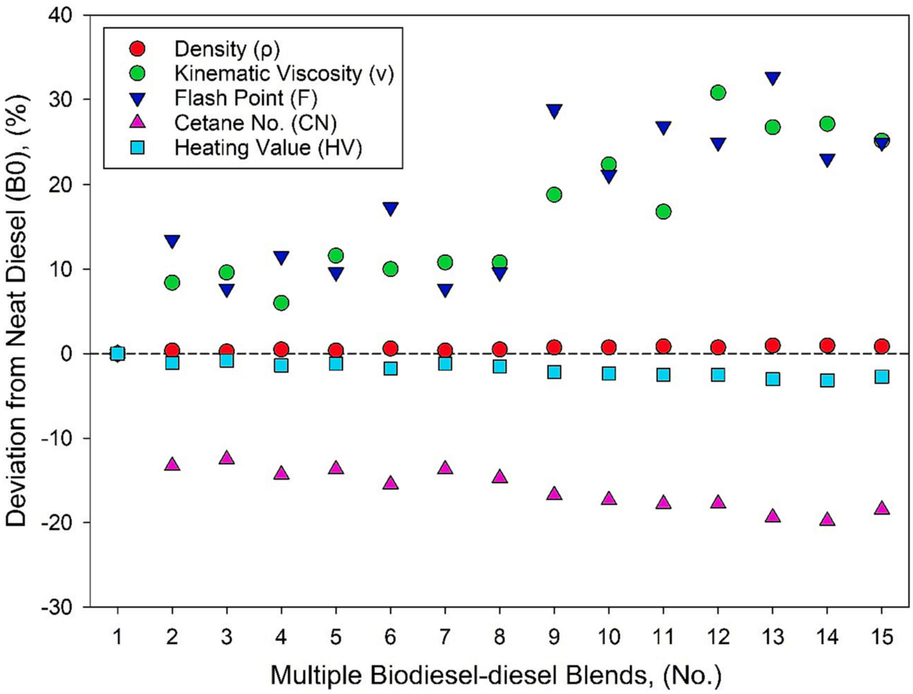

Fig. 4. Properties deviation from neat diesel (%) for multiple biodiesel-diesel blends.

test-rig [39,40]. Fig. 1 **and** Fig. 2 shows the schematic diagram and real photograph of engine test-rig. Exhaust emission is measured by using Netel make exhaust gas analyser with different sets of condition as mentioned above. The Netel make MGA-2 gas analyser measures the most common exhaust gas emissions such as NOx, CO, CO_2, and HC. Technical specifications DICI engine test-rig and the exhaust gas analyser are mentioned in the Table 4 and Table 5.

2.3. *Artificial neural network (ANN) approach*

Researchers need an option to traditional approaches and methods owing to their lack of ability in prediction [40]. The artificial neural network (ANN) simply designated as neural network (NN) is getting attention and has diversified applications in the field of engineering and medical sciences. ANN provides results based on various parameters

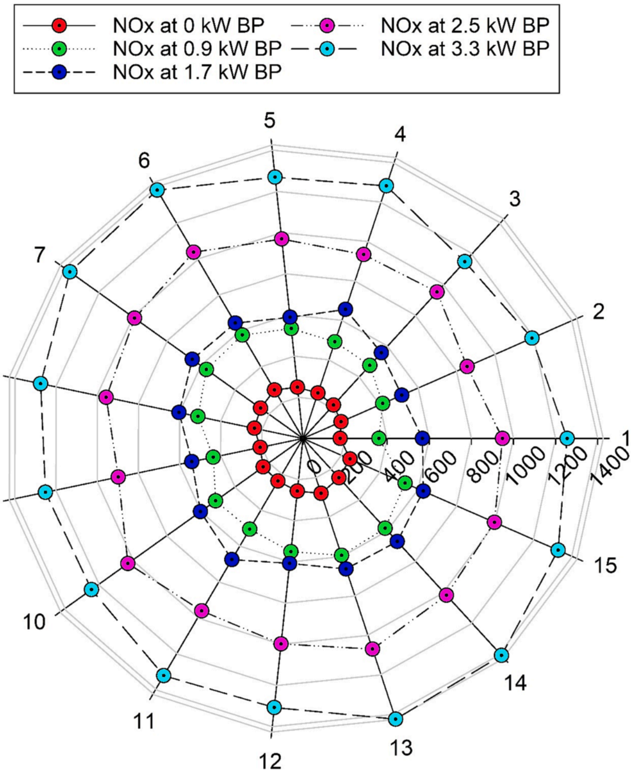

Fig. 5. Experimental NOx (ppm) for multiple biodiesel-diesel blends.

such as the number of hidden layers, number of neurons in the hidden layers, learning rate, momentum and activation factor may be varied until the network yields good predictions [33]. The application of ANN modeling is also applicable to IC engines for the evaluation of performance and emission characteristics. The neural network is consist of three layers viz: input, hidden, and output. In addition to this, the success of the algorithm is also dependent on user dependant parameters, learning rate and momentum constant. Standard algorithms used in ANN are back propagation, conjugate gradient, quasi-newton, and Levenberg-Marquardt (LM). Back propagation is a popular algorithm which has different variants such as gradient descent and gradient descent with momentum are often too slow for practical problems because it requires small learning rates for stable learning [37]. This disadvantages are eliminated by changing the weights. LM method is in fact an approximation of the newton's method. The algorithm uses the second-order derivatives of the cost function so that better convergence behaviour. LM technique extracts more significant parameter change vector and the error during learning is called as root-mean squared (RMS) [36]. ANN modelling was applied using feed-forward back-propagation neural network type with TRAINLM (Levenberg-Marquardt backpropagation) and LEARNGDM (Gradient descent with momentum weight and bias learning function) as a training of data and adaptation learning function. Two layers were utilized with 10 number of neurons by performing TANSIG (Hyperbolic tangent sigmoid transfer function) and PURLIN (Linear transfer function) transfer function in layer 1 and layer 2. The data set was arbitrarily divided into 3 categories with percentages of contribution to training (70%), validation (15%) and testing (15%). The algorithm makes the use of supervised training techniques in which the weights and biases are assigned random initial values in training phase. Each input was contributed equally in the training phase by pre-processing and scaling within the range of −1 to 1. Gradient descent rule was used for achieving error minimization and mean squared error (MSE) used as a performance function [41]. In present era of the research, the researchers always try to compare a parallel techniques alternative to classical one [40]. Intricate engineering problems receive robust solutions by utilizing viable techniques ANN [35]. NOx emissions are optimized by using ANN toolbox with the operating procedure defined by [42] and ρ, ν, F, and HV considered as a function. Fig. 3**.** Shows the architectural structure of ANN.

2.4. Uncertainty analysis

Three runs of test were performed under identical conditions to check for the repeatability of all the results. In general, the repeatability of the results was found to be within 2%. Each reading of the basic quantities measured is the average of three values. Errors and uncertainties in the experiments can arise from the instrument selection, condition, calibration, environment, observation, readings, and planning of the tests. Uncertainty analysis is needed to prove the accuracy of the experiments. An uncertainty analysis was carried out using the KLINE and McCLINTOCK (1953) [43].

If the result is dependent on 'n' independent variables of $x_1, x_2, x_3, \cdots, x_n$ then,

$$R = f(x_1, x_2, x_3, \cdots, x_n) \tag{1}$$

Then uncertainty 'w' in measurement of 'R' is given by.

$$w_R = \left[\left(\frac{\partial R}{\partial x_1} w_1\right)^2 + \left(\frac{\partial R}{\partial x_2} w_2\right)^2 + \cdots + \left(\frac{\partial R}{\partial x_n} w_n\right)^2\right]^{\frac{1}{2}} \tag{2}$$

Where,

$x_1, x_2, \cdots, x_n = Independantvariables$

$w_1, w_2, \cdots, w_n = Absoluteuncertainty$

$w_R = Uncertaintyintheresults$

Percentage uncertainties are observed 5.77% using KLINE and McCLINTOCK formula.

3. Results and discussion

3.1. Blends preparation and characterization

The physicochemical and thermal properties are found closer to the neat diesel for the blends under considerations. The variations in percentage deviations of properties from neat diesel are shown in Fig. 4. Few of the properties like flash point, viscosity are observed significantly higher whereas density found marginally higher than neat diesel fuel. Similarly, cetane number found significantly lowered whereas heating value found marginally lowered than that of neat diesel fuel. Density + 0.96% higher for blend No. 13 and 14 and an average increment observed + 0.58% for all multiple biodiesel/diesel blends. Similarly viscosity and flash point observed + 30.80% and + 32.69% higher than that of neat diesel and average + 15.68% and + 17.31% increment seen in the considered blends. On other hand significant reduction seen in cetane number −19.80% whereas −3.16% marginal reduction in heating value observed for the blend No. 14 and an average −15.84% and −1.84% reduction seen in cetane and heating value. The cetane number and the heating value of biodiesel blends decreased due to the unsaturation and self-oxygenation of the biodiesel.

3.2. Discussion on experimental oxides of nitrogen (NOx)

Higher amount of fuel is injected through the injector nozzle of the engine to achieve same power this happens because of higher viscosity and density of biodiesel concentration present in the blended fuels [39]. Lower heating value and higher amount of injected fuel increases the engine mean gas temperature, this attribution leads to increase the NOx emission of the engine [40]. NOx increases with increase in the Brake

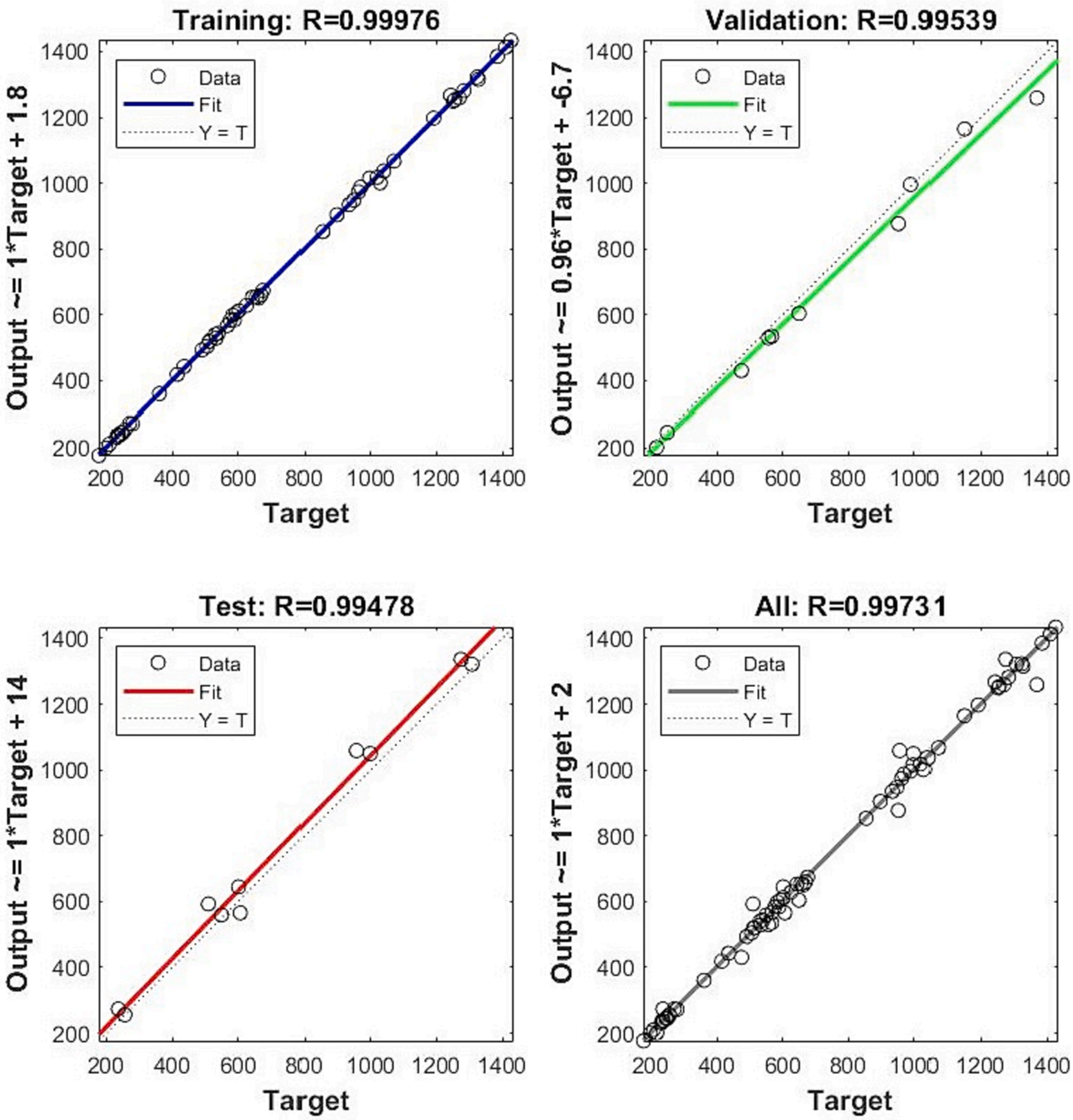

Fig. 6. Training, validation, and testing of NOx in ANN model.

powers (BPs) of the engine for multiple biodiesel/diesel blends under considerations. The highest NOx 1426 ppm observed for blend No. 13 whereas 1149 ppm observed for blend No. 3 at 3.3 kW BP. Fig. 5 shows the variations in experimental (Exp.) NOx of multiple biodiesel/diesel blends.

3.3. Discussion on estimation of NOx using ANN model

To the authors knowledge numerous authors have estimated engine characteristics from speed (rpm), mixtures or blends [44], and loading conditions [45]. The present research work focused on estimation of NOx using physicochemical and thermal properties as a function. Fig. 6 provides the comparison of results and data sets fittings for different parameters such as training, validation, and testing as $R = 0.99976$, $R = 0.99539$, and $R = 0.99478$ respectively. Further comparison of all parameters showed an accuracy of $R = 0.99731$ based on output and targets.

Fig. 7 illustrates the comparison of estimated (Est.), developed through ANN and experimental (Exp.) values of NOx for blends under considerations. Marginal variations in NOx is observed when estimated through ANN and experimental. The absolute error is observed as less than 1%.

Fig. 8 illustrates the deviation of estimated NOx (ppm) compared to neat diesel (B0) blend. Significant variations in estimated NOx of multiple biodiesel-diesel blends compared to neat diesel observed in four blends such as blend 3 (+75 ppm) at 2.5 kW BP, blend 7 (+109 ppm) at 3.3 kW BP, blend 8 (-102 ppm) at 2.5 kW BP and blend 12 (-51 ppm) at 2.5 kW BP. Remaining 11 blend of multiple biodiesel-diesel have shown average % variations within the range of −4% to + 5% compared to neat diesel. This increment of NOx emission have been observed due to increment of mean gas temperature of the engine. Highest density and viscosity of crude oil than the biodiesel and diesel fuel leads to increase in injection pressure and temperatures.

4. Conclusions

The experimentation has been performed on DICI engine with constant speed and CR with varying load, and with the help of ANN model NOx predicts from physicochemical and thermal properties. Following conclusions are drawn from experimental and computational investigations:

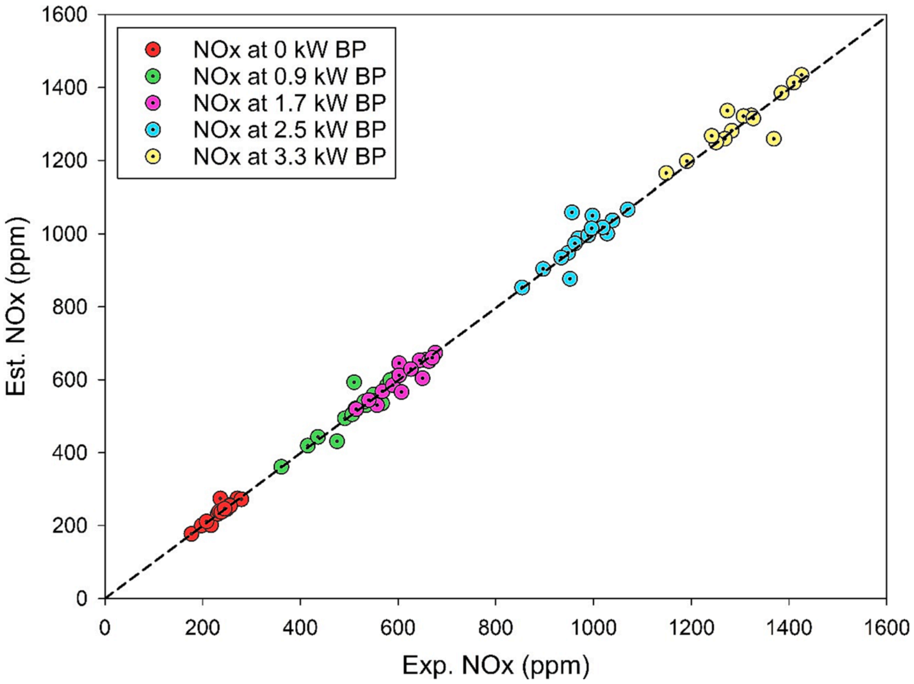

Fig. 7. Comparison of Exp. and Est. NOx (ppm).

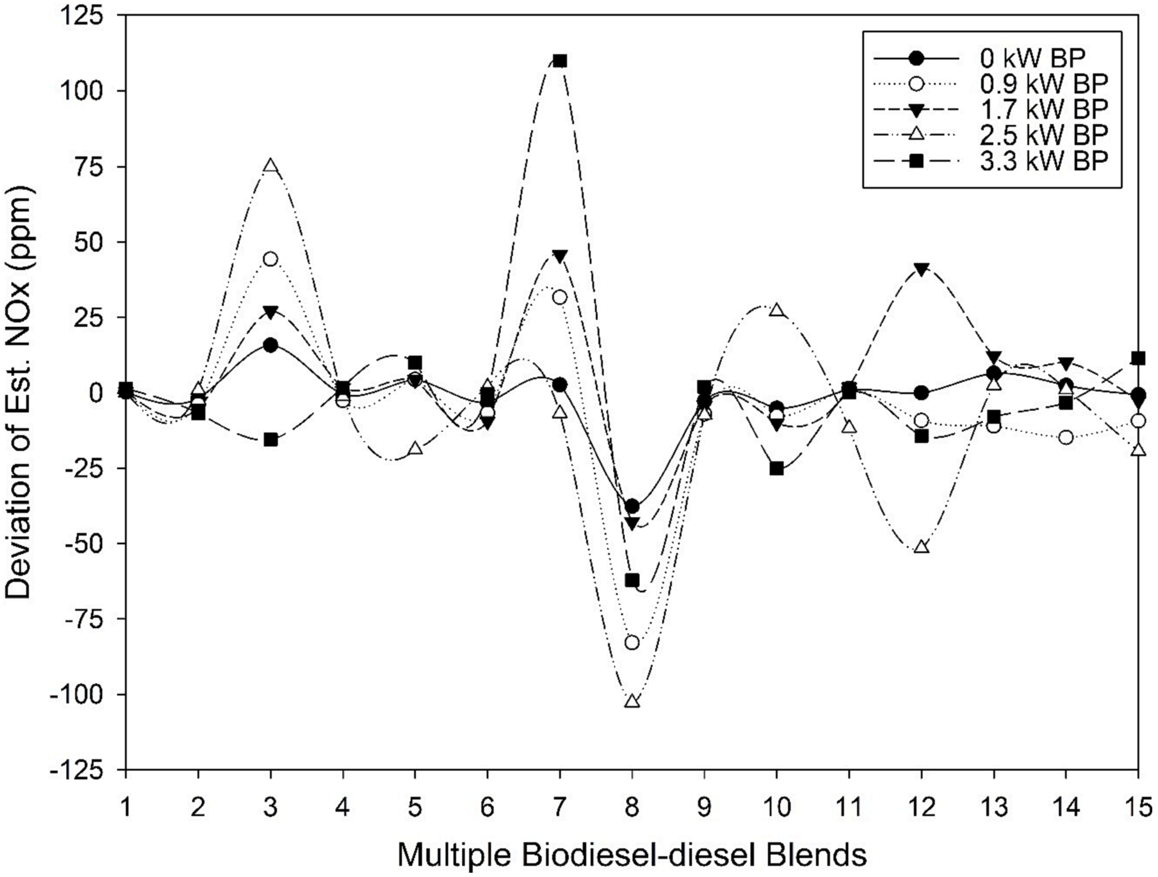

Fig. 8. Deviation of Est. NOx (ppm) for multiple biodiesel-diesel blends

- The density and viscosity of the blends rise as the concentration of biodiesel increases, whereas the cetane number and heating value decrease due to unsaturation and self-oxygenation of biodiesels.
- The concentration of biodiesel in blending plays a crucial impact in increasing oxides of nitrogen (NOx) emissions.
- Oxides of Nitrogen (NOx) increases as biodiesel content, braking power, and cylinder temperature increase.

- The oxygenation property of biodiesel and mean gas temperature of the engine increases as the proportion of biodiesel in the blends increases, resulting in an increase in NOx emissions.
- Highest and the lowest NOx observed as 177 and 1406 ppm at 0 kW and 3.3 kW BP for blend 1 and 13.
- Average increase in NOx observed as 18.93% compared to neat diesel.
- ANN model predicts Est. NOx with an accuracy of R = 0.99.
- The present study has been conducted on low speed engine, a long term test and high speed engines should be required to get more specific results of NOx emissions.

Declaration of Competing Interest

The authors 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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