Development of database and mathematical models for predicting engine performance parameters using biodiesel

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Abstract: A database for complete and quick knowledge of biodiesel was developed in Microsoft access linked with interactive interfaced of Visual Basic which contains various information such as biodiesel properties, engine performance parameters and emission characteristics. The comparisons of fuel properties among the biodiesel, its blends and engine performance parameters are one of the most attractive features of the developed database. Based on the data collected from the developed database, the analysis of variance (ANOVA) was carried out to know the effect of fuel properties on engine performance parameters. The fuel properties such as a change in calorific value and viscosity with respect to diesel were found to be significant at 5% level with brake power (BP) and brake specific fuel consumption (BSFC). However, flash point and density were found to be insignificant. Therefore, mathematical models were developed for (i) change in BP and (ii) BSFC based on the significant fuel properties. The model efficiency for BP and BSFC were found to be 92% and 91% respectively. The RMSE values were also calculated from the predicted value and found to be 1.85 and 5.45 for BP and BSFC respectively. From the above statistical facts, it is revealed that the developed mathematical models can be used to predict the change in BP and BSFC. Further, it is also expected that the developed database shall be expedient for researchers and engineers to locate various information related to biodiesel.

Keywords: biodiesel, engine performance, database, mathematical models, brake power, BSFC

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1 Introduction

The scarcity of known petroleum reserves makes renewable energy resources more attractive. The most feasible way to meet this growing demand is by utilizing alternate fuel sources. Biodiesel is one of the best candidates as an alternate fuel in diesel engines. The various fuel properties like density, kinematic viscosity, calorific values, flash point etc. are directly responsible factors for the efficient and smooth running of the engine. In recent decades, many researchers worked on different biodiesel such as Jatropha[1-7], Karanja[8-14], Coconut[15-17], Cotton[18-21], others biodiesel[22-29] and reported the properties of fuel and their blends. These properties are important to compare with diesel before conducting the engine performance tests. Further, comparison of fuel properties and their blends among different biodiesels are also vital. In the recent past, limited attempts[30-32] were made to compile the available information of different fuels and their blends together. In the absence of this compiled information, a significant portion of research

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work is to be devoted to collect the information from different published papers. This necessitates a computer based user-friendly database of fuel properties and their corresponding engine performance parameters. By getting the comparative performance of different fuels and blends, a further research plan can be formulated in these areas without conducting exhaustive review work.

Further, the researchers are interested in knowing the performance of the C.I. engine for various proportions of biodiesels and blends. It is complex, time consuming and costly to investigate the engine performance experimentally. A mathematical model based on major fuel properties would be helpful to estimate the engine performance without conducting the exhaustive experiments. Mustafa et al.[33] and Shivakumar[34] have put their effort to develop the ANN-based engine performance model, but these are limited for the specific biodiesel as well as engine type.

In the light of the above contexts, the present study has been formulated to develop a user-friendly database for fuel properties and mathematical modeling for predicting the engine performance based on fuel properties irrespective of biodiesel and engine type with following specific objectives: 1) To develop database for different biodiesels properties and engine performance parameters in Visual Basic environment; 2) To develop mathematical models for predicting changes in brake power and brake specific fuel consumption with reference to diesel and its validation.

2 Development of database

2.1 Data collection

The data were collected by an exhaustive review of the published and unpublished scientific research work. All the available information of biodiesels are taken into consideration for developing the database in the present study. The biodiesels of main concern was Karanja, Safflower, Palm, Rapeseed, Cottonseed, Coconut and Jatropha. Information such as (i) scientific classification (production, country and state wise) (ii) chemical properties (arachidic, gadoleic, linoleic, myristic, oleic, palmitic, palmitoleic, stearic, lauric, behemic and lignoceric) (iii) Fuel properties (calorific value, flash point, pour point, kinematic viscosity, density, refractive index and cetane index) and (iv) engine performance (brake power, brake specific fuel consumption, brake thermal efficiency and exhaust gas temperature) were collected for each biodiesel and their blends. These data of the biodiesels were fed into a database of Microsoft access and same can be read in systematic ways as and when required through a developed program in Visual Basis environment which has very interactive user interface.

2.2 Overview of the developed program

The overall approach described in this paper involves development and use of computerized simulation model for different biodiesel fuels. The software was developed in visual basic environment containing windows, a graphical user interface (GUI), which makes the software easy to use and understand. The software was developed in such a manner that novice user (without prior knowledge of software) can also run with the help of getting information from the help menu. The help menu guides the user in the proper execution, description of the software and its content available in the help menu. Software consists of several windows serving specific purposes such as databases for production related information, chemical properties, trans-esterification process, fuel, blend properties, engine performance parameters and so on. User can add, update or remove data from databases. The software has provision to export and save desired information in spreadsheet and text formats. The overall graphical representation of the developed program is shown in Figure 1.

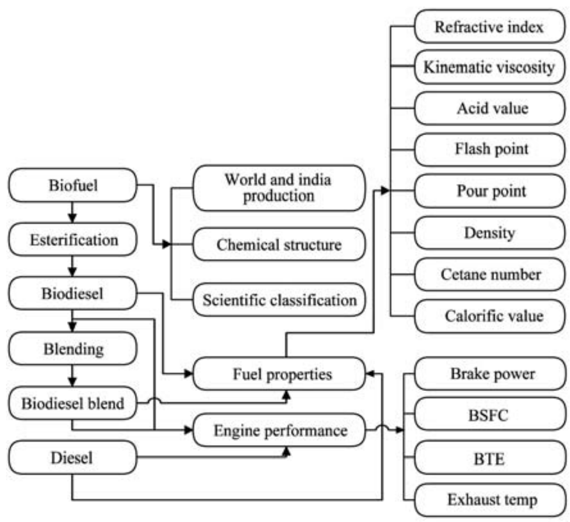


Figure 1 Flow chart to access the data through the developed program

2.3 Functioning of the software

The first window of the developed program is shown in Figure 2. On pressing the 'Select Fuels' button, the various fuels list appears on the window. In this window the type of fuel can be chosen from the drop down menu to view the database on the fuel. The flowchart for the production of biodiesel can be seen by selecting the 'Production Process' button. The components which play a major role in the production of biodiesel are stated under the 'Basic Component'. This also includes the description regarding the feedstock, alcohol, catalyst and neutralizer. The blending methods are also included in the database, which are mainly splash, In-tank, In-line and Rack. This can be viewed by clicking button 'Type of Blending'.

After selecting a particular oilseed second window appears which contains five menus Introduction, Chemical Structure, Oil Properties, World and India Production. These windows for cotton seed are shown in Figure 3.

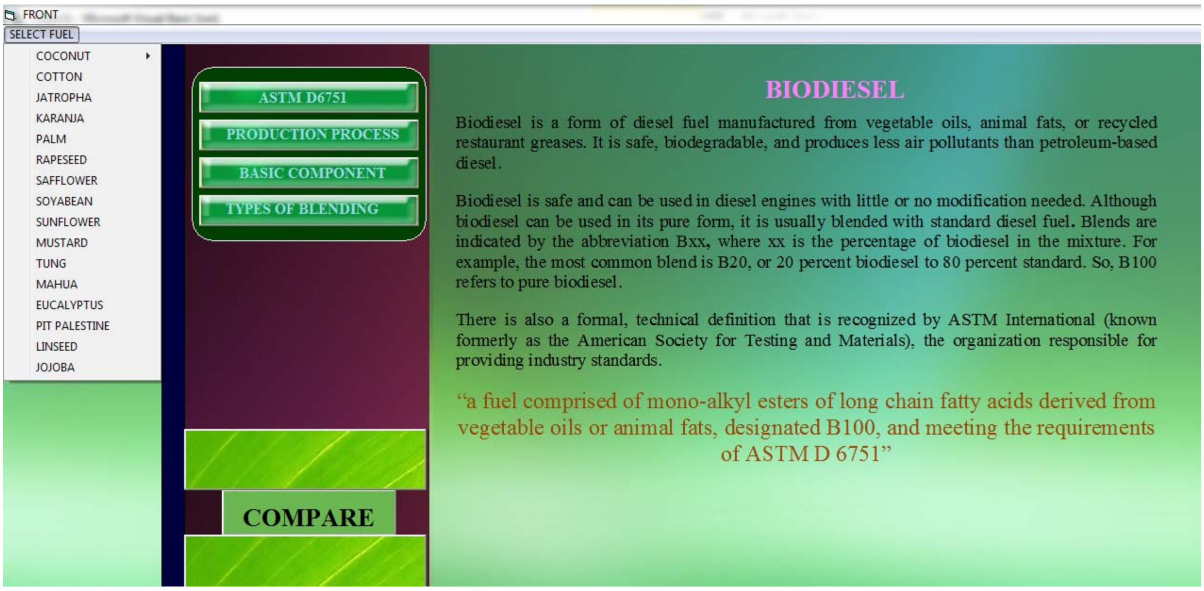
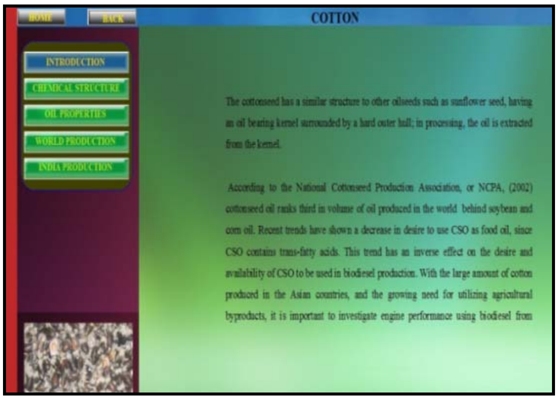
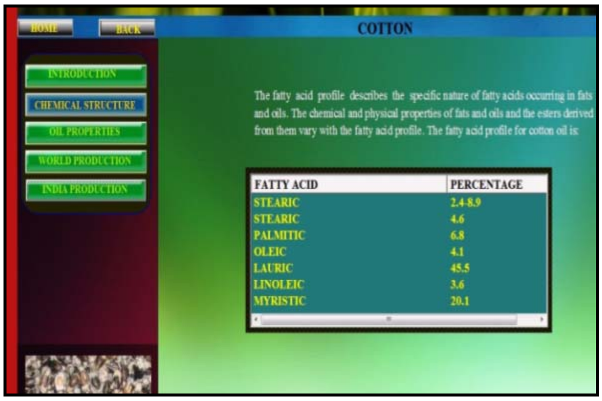


Figure 2 Front page of the developed program



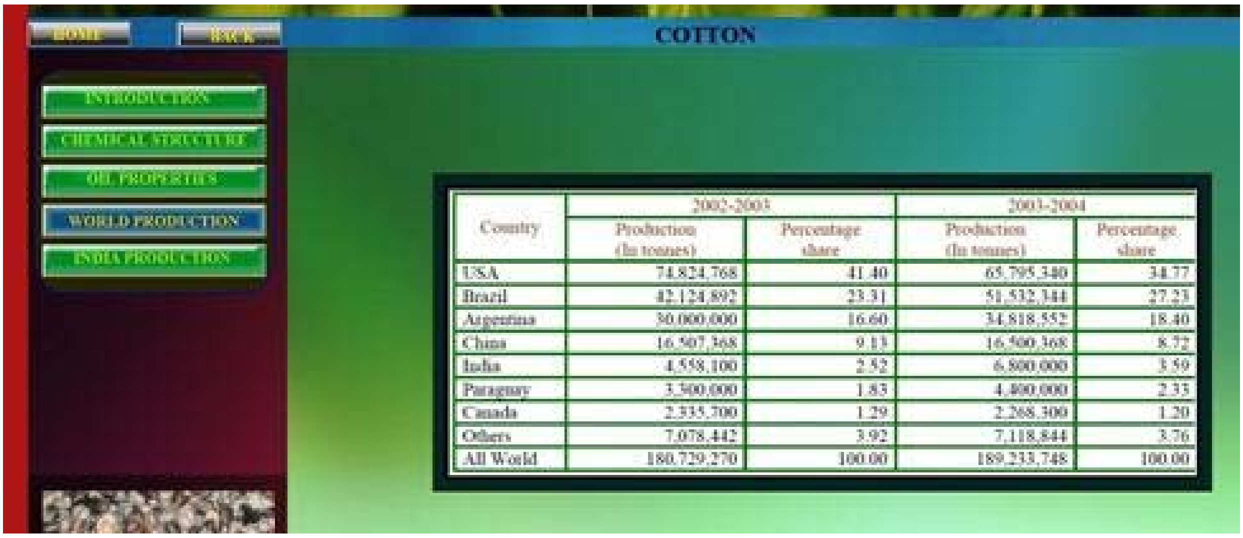
a. Introduction



b. Chemical structure

c. Fuel properties

e. India production



Country	2002-2003		2003-2004	
	Production (In tonnes)	Percentage share	Production (In tonnes)	Percentage share
USA	74,824,768	41.40	65,795,340	34.77
Brazil	42,124,892	23.31	51,532,344	27.23
Argentina	30,000,000	16.60	34,818,552	18.40
China	16,507,368	9.13	16,500,368	8.72
India	4,558,100	2.52	6,800,000	3.59
Paraguay	3,300,000	1.83	4,400,000	2.33
Canada	2,335,700	1.29	2,268,300	1.20
Others	7,078,442	3.92	7,118,844	3.76
All World	180,729,270	100.00	189,233,748	100.00

d. World production

Figure 3 Windows showing the different information of cotton seed

2.4 Comparisons of biodiesel

There are two different ways for the comparison in the developed program. First comparison can be done among the methyl ester of biodiesels which are obtained directly after esterification process. In order to make the comparison, click the "COMPARE" after selecting the preferable biodiesels. The fuel properties and engine performance parameters of the selected biodiesel will be displayed in the list box that is provided within the window (Figure 4a). Secondly, blend of one fuel can be compared with the blends of other biodiesels. This comparison is very much helpful, before going to conduct the engine performance test. The fuel properties and engine performance parameters of the selected blends appear in the list box (Figure 4b). Apart from the numeric comparison, a very good graphical comparison is also possible from the developed program. A graphical comparison of some of the fuel properties and engine performance is shown in Figure 5.

3 Development of mathematical model

3.1 Data collection and compilation

The following data were accessed from the developed biodiesel database and their blends, to develop mathematical models for brake power and brake specific fuel consumption. Further, similar information for diesels were also noted for respective research. The collected data were arranged in Microsoft Excel sheet for ease of access and further analysis.

1) Fuel properties of biodiesel and their blends:

i. Calorific value

ii. Flashpoint

iii. Kinematic viscosity

iv. Density

a. methyl ester of biodiesels

b. biodiesel blends

Figure 4 Comparison windows in the developed program

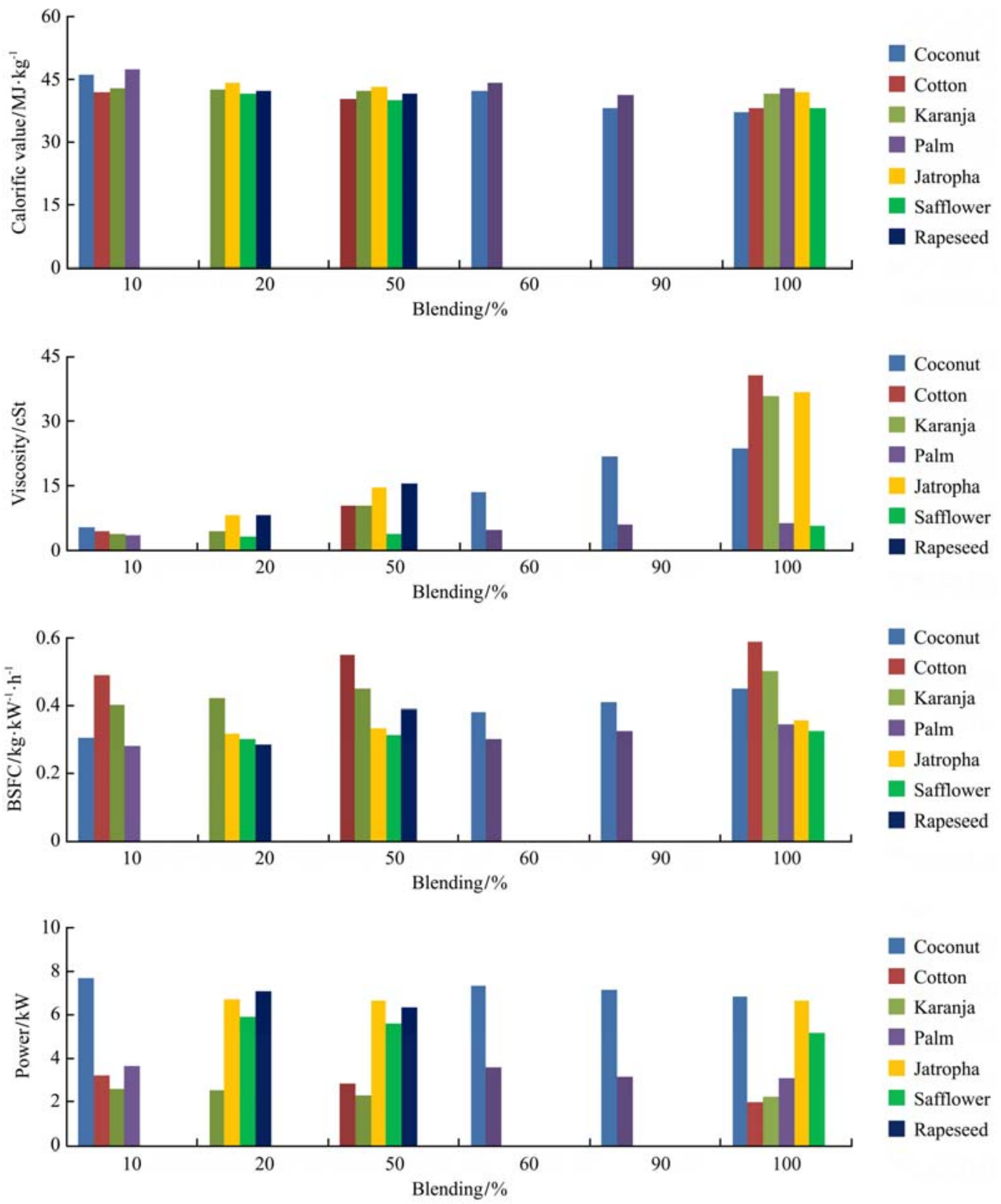


Figure 5 Graphical comparison of fuel properties and engine performance various biodiesel

2) Engine performance of biodiesel and their blends

i. Brake power

ii. Brake specific fuel consumption

The percentage change in the biodiesel properties with respect to diesel properties of the selected research work were calculated using Equation (1). It was observed that the diesel properties were different for different research work because of error involved in measuring method and the apparatus. The negative value shows the lower than diesel and positive means higher than diesel. Further, the changed in engine performance parameter with respect to particular engine was also calculated to eliminate the effect of engine parameters.

$$\text{Percentage change} = \frac{\text{Property of biodiesel} - \text{Property of diesel}}{\text{Property of diesel}} \times 100 \quad (1)$$

3.2 Analysis of variance

In order to check the effects of percentage changes in calorific value, viscosity, flash point and density on BP and BSFC, the analysis of variance was performed using SPSS statistical. Total 187 set of data were used to analyse the variance after proper checking and rectifying outlier in the collected data. The results of the test for BP and BSFC are shown in Tables 1 and 2, respectively. Table 1 indicates that the fuel properties such as change in calorific value and viscosity have significance on the brake power at 5% level as α is less than 0.05. However, the change in flash point and density were non-significant at 5% significance level because of α>0.05. Similarly, observations were also made from Table 2 that change in calorific value and viscosity have significance at 5% (α <0.05) level.

Table 1 Tests for effects for power between subjects

Source	Type III sum of squares	df	Mean square	F-value	Sig.(α)
ΔC*	499.627	1	499.627	56.986	0.000
ΔV*	435.243	1	435.243	49.642	0.000
ΔF	10.557	1	10.557	1.204	0.275
ΔD	1.034	1	1.034	0.118	0.732
Error	867.987	99	8.768		
Total	16236.272	104			
Corrected Total	5241.195	103			

Note: ΔC, ΔV, ΔF & ΔD – Percentage change in calorific value, kinematic viscosity, flash point & density; * Significance at 5% level.

Table 2 Tests for effects of BSFC between subjects

Source	Type III sum of squares	df	Mean square	F-value	Sig.(α)
ΔC*	8625.012	1	8625.012	232.675	0.000
ΔV*	518.397	1	518.397	13.985	0.000
ΔF	14.629	1	14.629	0.395	0.531
ΔD	89.601	1	89.601	2.417	0.123
Error	3669.816	99	37.069		
Total	36830.667	104			
Corrected Total	36771.165	103			

Note: ΔC, ΔV, ΔF & ΔD – Percentage change in calorific value, kinematic viscosity, flash point & density; * Significance at 5% level.

3.3 Model development

Mathematical models of BP and BSFC were developed for the engine performance parameters using multiple linear regression in SPSS statistical tool.

3.3.1 Brake power model

A multiple linear regression model was developed using SPSS for percentage change in brake power. The independent variables were percentage change in calorific value and viscosity. The results of model development are shown in Table 3, which indicates that viscosity and calorific values are significant with coefficients value of –0.011 and 0.604, respectively. The value for coefficient of determination, correlation and standard error of the developed model are 0.83, 0.91 and 2.9, respectively which are considered as an acceptable model. The developed model is given as:

$$\Delta BP = 0.604 \times \Delta C - 0.0108 \times \Delta V - 1.139$$

where, ΔBP = change in brake power, %; ΔC = change in calorific value, % and ΔV = change in viscosity, %.

Table 3 Coefficients of variables for power model

Model	Unstandardized coefficients		Standardized coefficients	t-value	Sig.
	B	Std. error	Beta		
Constant	–1.139	0.524	-	–2.173	0.032
ΔV*	–0.011	0.002	–0.467	–7.078	0
ΔC*	0.604	0.080	0.498	7.557	0

Note: Dependent variable: Power (*significance).

3.3.2 BSFC model

The results related to model development are presented in Table 4. The mathematical expression of the developed BSFC model is given as:

$$\Delta BSFC = -2.543 \times \Delta C + 0.011 \times \Delta V - 25.697$$

where, $\Delta BSFC$ = change in brake specific fuel consumption, %; ΔC = change in calorific value, % and ΔV = change in viscosity, %.

Table 4 Coefficients of variables for BSFC model

Model	Unstandardized coefficients		Standardized coefficients	t-value	Sig.
	B	Std. error	Beta		
Constant*	–25.697	1.084	-	–23.697	0
ΔV*	–2.543	0.166	–0.793	–15.361	0
ΔC*	0.011	0.003	0.187	3.629	0

Note: Dependent variable: BSFC (*significance).

The performance of the developed model was represented by correlation (r), coefficient of determination (R^2) and standard error which was found to be 0.94, 0.897 and 6.12, respectively. These values clearly signify that the developed model for the BSFC fit well.

3.4 Validation of the developed models

The developed models were validated with the data which were not used in the model development process. This was carried out by 15% of the total collected data. The validations of the developed models were evaluated with the help of Graph Pad Prism (GPP) software. For this purpose null hypothesis of equal variance and equal means at 5% level of significance with 29 degrees of freedom for change in power and BSFC were tested using F-test and t-test respectively.

The validation of models was also based on comparison of statistical parameters of simulated data with that of the observed data. The parameters used for model validation were Model Efficiency (ME) and Root Mean Square Error (RMSE). These parameters were calculated using following relationships:

$$ME = \left[\frac{1}{N} \sum_{i=1}^{N} (C_{si} - C_{oi}) \right]$$

$$RMSE = \left[\frac{1}{N} \sum_{i=1}^{N} (C_{si} - C_{oi})^2 \right]^{1/2}$$

where, ME = model efficiency; $RMSE$ = root mean square error; N = total number of data; C_{si} =i^{th} simulated data; and C_{oi} = i^{th} observed data.

The validation result of BP and BSFC models were represented in Tables 4. The calculated value of F-test and t-test were found less than critical value at that level of 5% significance and degree of freedom. Therefore, null hypotheses were accepted and it was concluded that simulated values of change in brake power and BSFC not differ significantly from observed value. F-test and t-test revealed the facts that developed models can be used for predicting the change in BP and BSFC by using the change in calorific value and viscosity of a particular biodiesel blend with reference to diesel fuel.

Table 4 Output of Graph Pad Prism for BP and BSFC model

Table analyzed	BP model	BSFC model
Observed power vs predicted power	-	-
Unpaired t -value	-	-
Are means significant different? (p<0.05)	No	No
One- or two-tailed p-value?	One-tailed	One-tailed
t, df	t=0.3593, df=56	t=0.2852, df=56
F-value to compare variances	-	-
F, DFn, Dfd	1.071, 28, 28	1.015, 28, 28
Are variances significantly different?	No	No

Further, Root Mean Square Error (RMSE) and Model Efficiency (ME) were calculated and found that ME is more than 90% for the both models. The RMSE of the BP and BSFC models are 1.85 and 5.45, respectively. These statistical values revealed that the developed model may be the good predictor of change in BP and BSFC.

The observed and predicted data were also plotted on 1:1 line to validate the developed models which are shown in Figures 6 and 7 for brake power and BSFC, respectively. A linearity pattern was observed in both the cases i.e. BP and BSFC with R^2 values of 0.9297 and 0.9076 respectively. These further strengthen the above statements that the developed models may be a good predictor for engine performance.

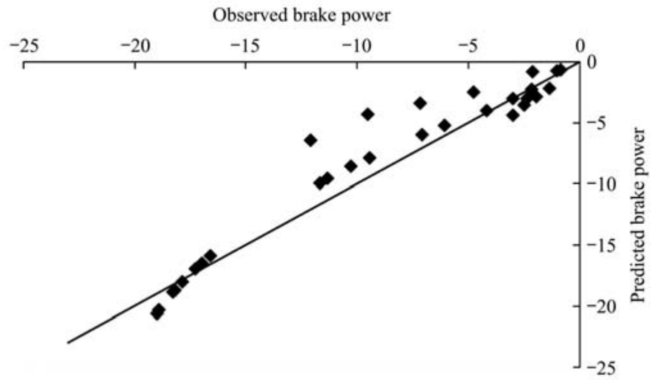


Figure 6 Plot of 1:1 between observed and predicted for brake power

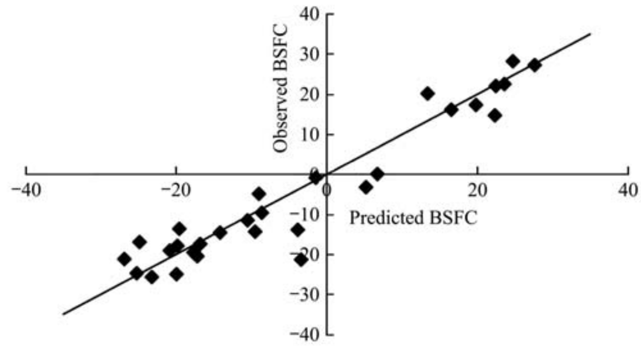


Figure 7 Plot of 1:1 between observed and predicted for BSFC

4 Conclusions

A user-friendly database for biofuels was developed which contains biofuel properties, engine performance parameters and emission characteristics. The comparison of fuel properties among the biofuels, biodiesel blends and engine performance parameters was one of the most attractive features of the developed database. Analysis of variance revealed that percentage change in calorific value and viscosity was found to be significant parameters with the percentage change in brake power and BSFC. The other fuel properties such as flash point and density were found to be non-significant. Mathematical models were developed for change in BP and BSFC based on significant fuel properties namely change in calorific value and viscosity. The model efficiency and RMSE for BP model were found to be 92% and 1.85, respectively. However, for BSFC model, they were 91% and 5.48, respectively. Therefore, it is also expected that the developed models will be useful to predict the BSFC and BP without conducting experiments.

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