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Prediction of cetane number and ignition delay of biodiesel using Artificial Neural Networks

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Abstract

This work deals with obtaining models for predicting the cetane number and ignition delay using artificial neural networks. Models for the estimation of the cetane number of biodiesel from their methyl ester composition and ignition delay of palm oil and rapeseed biodiesel using artificial neural networks were obtained. For the prediction of the cetane number model, 38 biodiesel fuels and 10 pure fatty acid methyl esters from the available literature were given as inputs. The best neural network for predicting the cetane number was a conjugate gradient descend (11:4:1) showing 96.3 % of correlation for the validation data and a mean absolute error of 1.6. The proposed network is useful for prediction of the cetane number of biodiesel in a wide range of composition but keeping the percent of total unsaturations lower than 80 %. The model for prediction of the ignition delay was developed from 5 inputs: cetane number, engine speed, equivalence ratio, mean pressure and temperature. The results showed that the neural network corresponding to a topology (5:2:1) with a back propagation algorithm gave the best prediction of the ignition delay. The correlation coefficient and the mean absolute error were 97.2% and 0.03 respectively. The models developed to predict cetane number and ignition delay using artificial neural networks showed higher accuracy than 95 %. Hence, the ANN models developed can be used for the prediction of cetane number and ignition delay of biodiesel.

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Key words: Cetane number, biodiesel, neural network, fatty acid, ester composition

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Nomenclature

ANN	Artificial neural network	BP	back propagation
CN	cetane number	CGD	conjugate gradient descend
ID	ignition delay	LM	Levenberg-Marquardt
FAME	Fatty Acid Methyl Esters	QP	quick propagation
n	engine speed [rpm]	QN	quasi-Newton
φ	equivalence ratio	DBD	Delta-bar-Delta
Pm	mean pressure	T	temperature in Kelvin
R	correlation coefficient		

1. Introduction

Energy is the most fundamental requirement for human existence and activities. As an effective fuel, petroleum has been serving the world to meet the needs for energy production and consumption [1]. But the fast industrialization of the world has led to an increase in the demand for petroleum-based fuels obtained from limited sources. To reduce the dependence on fossil fuel, researches on alternative fuels are being extensively carried out, especially on biofuels [2]. Biodiesel is one of the potential alternative fuels and has been widely used in many countries [3]. Biodiesel exhibits several advantages when it is compared to the existing petroleum fuels. It has physical properties near to the standard diesel and it is easily produced and is renewable. Biodiesel fuels are generally classified as fatty acid methyl esters (FAME), which are derived from the alkali-catalyzed trans-esterification of fats and oils with methanol, although other alcohols can be used [4].

Several physical properties of biodiesel fuels depend on their fatty acid ester composition [1-3]. Also related to the ester composition is the cetane number which is one of the most cited indicators of diesel fuel quality [3-5]. The CN of FAME fuels clearly vary with the degree of unsaturation. The literature also reports that increasing degree of unsaturation leads to decreasing CN [2], [6-9]. It is generally dependent on the composition of the fuel and can influence the engine stability, noise level, and exhaust emissions. While the ignition delay can be influenced by engine type and operation conditions, the cetane number mainly depends on the chemical composition of the fuel.

Some researchers have obtained models to predict the cetane number of diesel fuel or biodiesel, correlating this parameter with different input factors or using different mathematical methods. Cheenkachorn [3] developed statistical models and artificial neural networks for prediction of biodiesel properties from the fatty acid composition. Dongmei [10] developed a simple model for predicting CN of biodiesel from its FAME composition while Yang [11] developed multiple linear correlation equations for predicting the cetane number for 12 hydrocarbons in order to compare with a model developed using Artificial Neural Networks (ANNs). Others equations for cetane number estimation have been proposed. e.g. Bamgboye [12], Ramirez-Verduzco [8] and Saxena [13].

The cetane number of a fuel is related to the ignition delay time. The shorter the ignition delay time, the higher is the cetane number, and vice versa [2]. The ignition delay in direct injection diesel engines is of great interest due to its direct impact on the heat release, as well as its indirect effect on engine noise and pollutant formation. The ignition delay period is composed of a physical delay, encompassing atomization, vaporization, and mixing, coupled with a chemical delay, a result of pre-combustion reactions in the fuel/air mixture. The two time scales are occurring simultaneously [5].

Assanis [14], in a work developed for the ignition delay estimation, analyzed several papers that cover constant volume bombs, steady flow reactors, rapid compression machines and combustion engines. Several of those correlations use an Arrhenius type equation. Also Kadota et al. [14] performed a fundamental study of fuel droplet autoignition in an elevated pressure/temperature environment and showed that the ignition delay of hydrocarbon droplets can depend on the available oxygen content. Weisser et al. [14] took into account low, intermediate, and high temperature chemical processes for developing their ignition delay correlations.

Determination of the CN by an experimental procedure at present is an expensive and time consuming process. Therefore, the obtaining of accurate models to predict the cetane number of biodiesel from its Fatty Acid Methyl Ester composition in a wide range of feedstocks characteristics would be useful for the scientific community. On the other hand, the estimation of the ignition delay based on the use of ANNs can allow to decrease the absolute error brought by other correlations and increase the range of biodiesel fuels to be applied. Nevertheless, the ignition delay is a dynamic process mainly influenced by dynamic variables; therefore, the estimation of it using ANNs is an approach to be carefully studied and assessed before its implementation.

The scope of the investigation is to obtain models for the estimation of the cetane number and ignition delay of biodiesel using ANNs, seeking for the best suitable model to predict both in the range of biofuels studied.

2. Experimental set-up and procedures

In the present work 48 different biodiesel fuels (including 10 pure fatty acids) and their cetane numbers were taken from references as input and output data for the implementation of ANNs for predicting the cetane number. The main FAME composition presented in biodiesel obtained from different feedstocks is covered by ten input FAMEs selected [15],[16], [10, 17-22]. The input data covers FAME composition and the output covers the cetane number. The validation of the models obtained was done using a separate data set selected from literature reports, which was not used for developing the models. The data selected for validation covers 15 samples.

For the cetane number estimation, different networks were developed using five basic topologies, between (11:3:1) and (11:7:1). The ANNs used were the multilayer Perceptrons, with one hidden layer and five or seven units. The inputs of the network were ten, representing the chemical composition of 10 FAMEs and one input representing the total amount of the other FAMEs found in the biodiesel sample. 60 different ANNs were tested for the prediction of the CN. The experimental data used in the ANNs training step for cetane number estimation is shown in [23].The CN was the unique variable output of the network.

For the ignition delay, ANNs for palm oil and rapeseed oil biodiesel were also developed. The input variables were n, φ, Pm, T and CN; the output covers the ID. The input values are corresponding to engine tests in a direct injection diesel engine, except for the CN that was calculated through the best network for the CN (conjugate gradient descend, 11:4:1) and according to the composition of both biofuels. The engine tests were performed with two biodiesels (palm and rapeseed). The engine used was a four stroke diesel engine, type Volvo TD60B turbocharged with six vertical cylinders in an in-line arrangement and water cooled. Table 1 shows the main engine specifications and the valve timing and injection timing [5].

Table 1. Engine specifications

Feature	Values
Connecting rod length	0.23m
Bore	0098m
Stroke	0.12m
Compression ratio	16
Swept volume per cylinder	913.12cm^3
Total swept volume	5479 cm^3
Inlet valve opens 18	18° before TDC
Inlet valve closes	234° after TDC
Exhaust valve opens	120° after TDC
Exhaust valve closes	16° after TDC
Injection starts	22° before TDC

The experiments were performed at different torque (Me). The selected values were 138, 277 and 415 Nm, respectively, covering in this order low, medium and high engine loads. The engine speed was varied between 1500 and 2300 r/min [5].

For the determination of the start of combustion, the first derivative of in-cylinder pressure vs. crank angles degrees (φ) was used. The start of combustion was defined at the moment where the rate of pressure rise (dp/dφ) drastically changes. With the start of injection (22°ca before top dead center) and the start of combustion, the ignition delay is obtained for the different working conditions (load and engine speed). The temperature was calculated starting from experimental data of in-cylinder pressure and φ. The temperature was calculated according to a procedure previously developed [5, 24]. The basic neural network topology implemented for the ID model was (5:2:1). Also the typical multilayer Perceptrons were used. 12 ANNs were used for the prediction of ignition delay.

In the training step, two phases were established for both modelling processes (cetane number and ignition delay estimation), keeping constant the phase 1 (back propagation) for all the ANNs evaluated. The second phase was varied among different possibilities: back propagation, conjugate gradient descend (CGD), Levenberg-Marquardt (LM), quick propagation (QP), quasi-Newton (QN) and Delta-bar-Delta (DBD). The training was developed for 10000 epochs with a learning rate of 0.01. Linear and logistic functions in the range of 0.9 were used as the output functions among different networks. The approach to select the best network was based on the selection of the highest correlation coefficient and lowest absolute errors.

3. Results and Discussion

The search for the best network for predicting the CN and the ID was based on the lower absolute error as the objective function in the process, but combining it with adequate values of the correlation coefficient found. The results found for these two objective functions covering the whole group of ANNs in order to find the better CN and ID prediction are shown in Table 2, Table 3 and Table 4.

Table 2. Absolute errors and correlation coefficients (%) for the CN using a linear output function

ANNs	BP	CGD	DBD	LM	QN	QP
11:3:1	2.7 (94.7)	2.4 (93.5)	2.4 (94.9)	1.9 (94.6)	1.9 (95.1)	2.1 (95.9)
11:4:1	2.9 (93.4)	1.6 (96.3)	2.3 (94.3)	2.4 (93.0)	1.6 (95.7)	2.4 (94.6)
11:5:1	2.3 (93.9)	2.6 (94.9)	2.0 (95.3)	2.3 (95.2)	2.1 (95.9)	2.1 (95.0)
11:6:1	2.3 (93.9)	2.5 (94.3)	2.0 (93.5)	1.9 (95.0)	2.4 (92.4)	1.9 (95.7)
11:7:1	2.7 (94.0)	2.3 (94.9)	2.6 (92.6)	2.0 (95.8)	1.8 (95.4)	2.1 (94.3)

The results shown in Table 2 represent the absolute error and correlation coefficient for all the ANNs tested corresponding to the cetane number estimation, changing the phase two among six algorithms, varying the number of nodes between 3 and 7, using the linear output function. Table 3 shows the results for the same method and training algorithm but corresponding to a logistic output function.

Table 3. Absolute errors and correlation coefficients (%) for the CN using a logistic output function

ANNs	BP	CGD	DBD	LM	QN	QP
11:3:1	2.2 (94.0)	2.1 (94.4)	2.6 (93.5)	2.2 (95.4)	2.4 (94.2)	2.3 (94.8)
11:4:1	2.8 (93.0)	2.6 (93.1)	2.4 (92.9)	2.3 (94.8)	2.5 (94.1)	2.6 (94.2)
11:5:1	2.2 (93.3)	2.5 (94.8)	2.0 (92.9)	2.4 (93.8)	2.2 (95.7)	2.1 (96.1)
11:6:1	2.1 (92.4)	2.3 (94.2)	2.1 (93.3)	2.7 (94.0)	2.0 (94.3)	2.4 (92.6)
11:7:1	1.9 (94.8)	2.3 (93.5)	2.2 (91.1)	2.5 (91.0)	2.5 (93.1)	2.3 (91.0)

Table 4. Absolute errors and correlation coefficients (%) for ignition delay

ANNs	Function	BP	CGD	DBD	LM	QN	QP
5:2:1	Linear	0.04 (93.7)	0.04 (95.1)	0.04 (96.2)	0.05 (94.7)	0.05 (94.0)	0.04 (95.6)
5:2:1	Logistic	0.03 (97.2)	0.03 (96.8)	0.06 (93.4)	0.05 (94.3)	0.04 (96.4)	0.05 (94.0)

All the tables have shown the absolute errors and the correlation coefficients (in parenthesis). Concerning the cetane number, the critical point is that in several networks it is not possible to obtain absolute errors below 2, as is observed in Table 1. Only eight ANNs are below this value. However, for the ignition delay estimation the networks developed showed very low absolute errors joint to adequate correlation coefficients.

3.1 Models validation

The models validation was only developed for the cetane number. For the ignition delay estimation, the validation was not developed due to the low amount of experimental data collected; therefore, the use of a validation data set was in this case not possible. The authors of this work are considering the result of the estimation of ignition delay based on ANNs as preliminary results.

Two ANNs were selected for the validation step for the cetane number estimation, according to the lowest absolute errors combined with two of the highest correlation coefficients found. As can be observed in Table 2, the lowest absolute error values were obtained for CGD and QN algorithms (for the CN estimation). Therefore, for the validation step both networks were selected.

For the validation of the selected models, a data set not related to the modelling data was used [23]. The validation data covers 15 samples from other references. The collected data includes the experimental evaluation of FAME composition and the cetane number, covering a wide range of possible cetane

number values (between 41 and 69) and taken from experiments using engine tests or an ignition quality tester.

The prediction capability of the selected models for this external data were based on the comparison between the predicted cetane number (using ANNs) and the experimental value (actual value) trying to find less residuals for the whole data tested. A compendium of the main statistical results of the validation process corresponding to the selected models is shown in Table 5. The analysis of the networks showed that the prediction capability of the network using the CGD is better than using the QN algorithm. As is shown in Fig. 1, in many evaluated points, the prediction is better using the ANN (11:4:1) with a CGD algorithm than using the QN algorithm. This selection is also based on the sum of squares corresponding to the residual values on the cetane number estimation. The lowest sum of squares was also obtained for the CGD.

Table 5. Statistical results in the validation process

ANN	Function	Absolute Error	*R* for the validation data	Sum of squares
CGD (11:4:1)	Linear	1.6	96.3 %	150.3
QN (11:4:1)	Linear	1.6	95.7 %	196.0

According to the analysis exposed above, the best network is implemented using the topology (11:4:1) of 11 inputs, 1 output variable and four nodes. The response surface obtained for this CGD (11:4:1) network for the prediction of the CN as a function of Myristic and Lauric ethyl esters percents is shown in Fig.2. In the right side the plot of the Palmitoleic percent versus the CN values is shown. It was the only two-dimensional relationship obtained with changes in the CN influence depending of the factors magnitude (Palmitoleic percent).

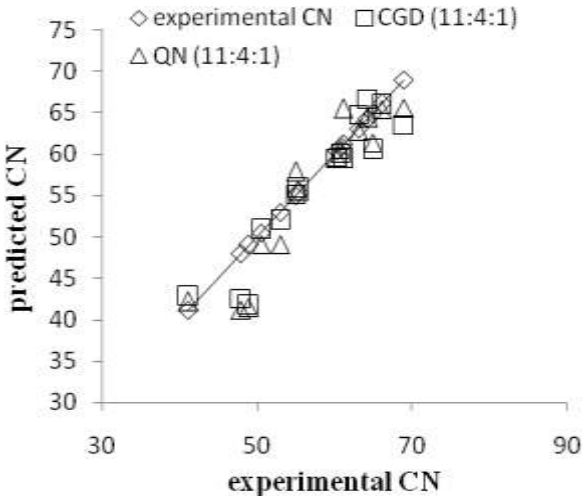

Fig. 1. Comparison between two ANNs for prediction of the CN

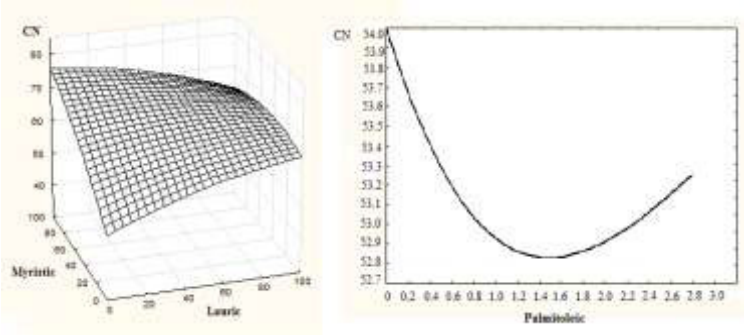

Fig. 2. Response surface and Palmitoleic percent influence in the CN estimation using a CGD (11:4:1)

Lack of accuracy was observed in certain cases of the validation step, when the total percent of unsaturations in the FAME composition of the biodiesel reach certain levels. As is observed in Fig.3, for higher values than 80 % in the total unsaturations, in some cases the uncertainty percent is increased, reaching values higher than 5 %.

According to Fig.3, even when some values are well predicted by one or both ANNs, the general behaviour is of low accuracies when the unsaturation percent is higher than 80 %, therefore the selected best model can fail in this critical range of total unsaturations. Under this range, the ANN (11:4:1) with CGD algorithm predicts the cetane number with equal or higher accuracy than 95 %. The model is not recommended for predicting cetane number of pure FAMEs different from the selected ones for this work.

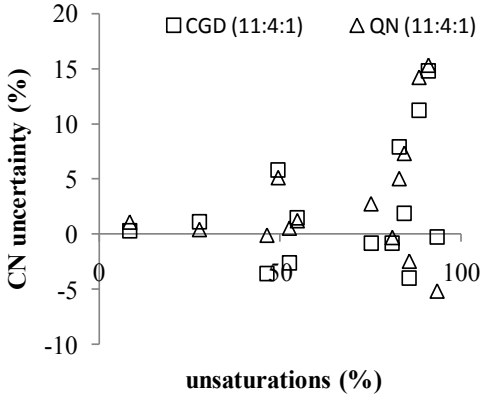

Fig. 3. Uncertainties percent vs. unsaturation percent for the selected ANNs

Yang [11] used a backpropagation neural network model with a training step and a validation step. Ramadhas [4] used an ANN to predict cetane number selecting four types of networks. Basu [25] also used backpropagation, Levenberg, quick propagation and delta-bar-delta as training algorithms in three layer (8:3:1) neural networks. For diesel fuels, he found correlation values for the network in the training

step (R = 0.9539). Yang [11] obtained R = 0.8602 for the training step in a three layer backpropagation network with 2.1 for the mean absolute error but his network is only applied to diesel fuels.

Ramadhas [4] used four types of ANNs, not reporting the absolute error of the networks. The author used 5 inputs corresponding to 5 FAME while in this work it is extended to 11 inputs. Ramadhas used a data set that covers biofuels with cetane number between 22.7-75.6, similar to the range applied in the present work. Therefore the prediction capability of their ANNs can only be restricted to the composition of 5 FAMEs that is quite limited due to the amount of feedstocks, different in chemical composition that can be found in these biofuels.

Conclusions

Two models have been proposed to predict the cetane number and ignition delay using artificial neural networks respectively. The ANNs used were the multilayer Perceptrons for both model. An artificial neural network model was developed to predict cetane number of biodiesel from their fatty acid composition. The best neural network for predicting the cetane number was a backpropagation network (11:4:1) using a Conjugate Gradient Descend algorithm for the second training step. The model yielded an *R* value of 96.3 % and a mean absolute error of 1.6 for the validation data. Also using ANNs, a model for the ignition delay prediction based on two biodiesels (palm and rapeseed) data sets was developed. The network selected to predict the ignition delay was a (5:2:1) with a correlation coefficient of 97.2 % and an absolute error of 0.03. The proposed networks are useful for prediction of the cetane number and ignition delay of biodiesel fuels.

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