Revista Cubana de Ingeniería Vol. X (3) 34-45 (2019) ISSN: 2223-1781

Artículo Original

Assessment of the prediction capability of biodiesel cetane number by Artificial Neural Networks

Ramón Piloto-Rodríguez[1,*], Yisel Sánchez-Borroto[1], Eliezer Ahmed Melo-Espinosa[1]

[1]Universidad Tecnológica de La Habana "José Antonio Echeverría" (CUJAE). Calle 114 No. 11901 entre Ciclovía y Rotonda, Marianao, La Habana, Cuba.
*Corresponding author: rpiloto@ceter.cujae.edu.cu

Este documento posee una licencia Creative Commons Reconocimiento/No Comercial 4.0 Internacional

Recibido: 17 noviembre 2019 **Aceptado:** 20 diciembre 2019 **Publicado:** 17 febrero 2020

Abstract

Artificial Neural Networks for the estimation of the cetane number of biodiesel from their fatty acid methyl ester composition were evaluated in this work. The study covered 64 neural networks varying the number of nodes in the hidden layer and using five topologies and six different algorithms for the second training. An experimental data from literature reports that covers 48 and 15 biodiesels in the modeling-training step and validation step respectively were taken. After the training step, the best two ANN concerning selected statistical parameters were used in a validation step, using an external data. A model to predict cetane number using an artificial neural network was obtained with better accuracy than 95%. The best neural network to predict the cetane number was a backpropagation network (11:4:1) using the Conjugate Gradient Descend algorithm for the second step of the networks training and showing 93.8% of correlation. The proposed network is useful for prediction of the cetane number of biodiesel in a wide range of FAME composition but keeping the percent of total unsaturation lower than 80%.

Keywords: cetane number, biodiesel, neural network, fatty acid, ester composition

Nomenclature

CN cetane number	*M* percent of Myristic
ASTM American standard	*P* percent of Palmitic
ANN artificial neural networks	*Pt* percent of Palmitoleic
CFR Cooperative Fuel Research engine	*S* percent of Stearic
IQT ignition quality tester	*O* percent of Oleic
R^2 coefficient of determination	*Li* percent of Linoleic
FAME fatty acid methyl esters	*Ln* percent of Linolenic
MLR multiple linear regression	*Ei* percent of Eicosanoic
BP backpropagation	*Er* percent of Erucic
CGD conjugate gradient descend	*Ot* sum of residual FAME to reach 100%
QP quick propagation	Wt weight percentage
BD biodiesel	*R* coefficient of correlation
La percent of Lauric	

1. Introduction

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 [3-9]. The cetane number measures the readiness of the fuel to autoignite when it is injected into the combustion chamber. It is generally dependent on the composition of the fuel and can influence the engine stability, noise level, and exhaust emissions.

The cetane number (CN), determined by a standard diesel engine is a measure of the ignition quality of a diesel fuel in a compression ignition engine. A fuel with higher cetane number has a shorter ignition delay period and starts the combustion shortly after it is injected into the chamber [4]. 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. The cetane number of biodiesel is generally higher than the standard diesel fuel. Experimental data shows values varying between 45-67 for biodiesel and ranged between 40-49 for diesel fuel [10, 11]. A single fatty acid alkyl ester molecule can have a cetane number between 42-89, depending on its molecular structure [10]. Van Gerpen [10] studied the effect of adding pure esters to diesel fuel using a linear regression fit on the CN data for each ester as a function of the percent of ester in the blend.

Equations for predicting the cetane numbers of diesel or biodiesel fuels have been published [4, 12-18], correlating this parameter with different input experimental factors or using different mathematical methods. Yang [12] developed multiple linear correlation equations and artificial neural networks (ANN) for predicting the CN for 12 hydrocarbons. Most of the models published for cetane number prediction were developed with Multiple Linear Regression (MLR) techniques. That procedure requires the user to specify a priori a mathematical model to fit the data in order to obtain the empirical correlation. An alternative to avoid that problem is the use of artificial neural networks.

Unlike the correlation techniques, the neural network can identify and learn the correlative patterns between the input and output data once a training set is provided. The use of ANN for predicting and modeling of energetic and mechanical systems is reported [19-26]. Their use in the modeling of engines combustion processes is also reported [27-30]. Very few works reported the use of ANN to predict cetane number of diesel fuels [12, 31, 32], and only one for its prediction in biodiesel fuels [15].

Yang [12] used a backpropagation neural network model with a training step and a validation step. The results shown a higher coefficient of determination (R^2 = 0.97) than using MLR. Basu [31] obtained relationships between the CN of diesel fuels using nuclear magnetic resonance. The cetane number was determined using an IQT. Ramadhas [15] used an ANN to predict cetane number selecting four types of networks. Santana [32] estimated the CN of individual components of diesel fuel using ANN. The neural networks have also been applied to the prediction of other fuel properties [33].

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 CN of a biodiesel from its FAME composition in a wide range of feedstocks characteristics would be useful for the scientific community. The modeling of CN based on ANN brings more advantages than the use of linear regression because opens the possibility of the use of networks ensembles for prediction of more complex parameters. One example is the prediction of the ignition delay, that depends on several related factors and one of them is the cetane number.

The purpose of this work is to obtain good performance ANN for predicting the cetane number of biodiesel from its FAME composition, when different parameters of the network are varied. This study covers changes in the network topology, training algorithms and learning rate, seeking for the least mean absolute error in the prediction.

2. Experimental set-up and procedures

In the present work 48 different biodiesel fuels (including 10 pure fatty acids) were taken from references as input and output data for the obtaining of ANN for predicting the cetane number. The FAME main composition presented in biodiesel obtained from different feedstocks is covered by ten FAME selected [13, 15, 18, 34-39]. 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 validate covers 15 samples. The degree of relationship between measured and fitted cetane number data was expressed as the R and R^2. The best fit was expressed as the higher R and the lower mean absolute error.

Several networks were developed using different topologies from (11:3:1) to (11:7:1). The only difference with the others is in the number of neurons in the hidden layer. The ANN used were the multilayer Perceptrons, with one hidden layer and between 3 and 7 units. The inputs of the network were ten, representing the chemical composition of 10 FAME and one input representing the total amount of the other FAME found in the biodiesel sample. The CN was the unique variable output of the network.

The chemical formula and the structure of the FAME on which this research is focused are shown in Table 1. The ten FAME listed represent the inputs for the CN modeling. The basic structural description for the input FAME used in this work (XX:X) covers the information about the number of carbon atoms (XX) and the number on the right (X) represents the number of unsaturation in the molecule.

In the training step two phases were implemented, keeping constant the phase 1 (back propagation) for all the ANNs evaluated. The training was developed for 10000 epochs with a learning rate of 0.01. Linear and logistic functions were used as the output functions in different networks variants. In the search for the neural network that brings short absolute error in the estimation of cetane number joint to lower correlation coefficients. The learning rate was kept constant at 0.01 and not varied due to the known direct proportionally dependence of the mean square error and the learning rate [40]. Therefore the learning rate was kept as lower as possible.

Table 1. Chemical structure and name of the FAME

Fatty acid	Structure	Formula
Lauric	12:0	$C_{12}H_{24}O_2$
Myristic	14:0	$C_{14}H_{28}O_2$
Palmitic	16:0	$C_{16}H_{32}O_2$
Palmitoleic	16:1	$C_{16}H_{30}O_2$
Stearic	18:0	$C_{18}H_{36}O_2$
Oleic	18:1	$C_{18}H_{34}O_2$
Linoleic	18:2	$C_{18}H_{32}O_2$
Linolenic	18:3	$C_{18}H_{30}O_2$
Eicosanoic	20:1	$C_{20}H_{38}O_2$
Erucic	22:1	$C_{22}H_{42}O_2$

60 different ANN were tested for the prediction of the CN. The ANN used two phases in the training step. The phase one was a backpropagation (BP) and the second phase was varied among different possibilities: back propagation, conjugate gradient descend (CGD), Levenberg-Marquardt, quick propagation (QP), quasi-Newton and Delta-bar-Delta. The experimental data used for training the ANN shown in Table 2. Twelve ANN (for each topology) were evaluated keeping constant the function for phase 1 (back propagation) and changing phase 2 and the regression output function.

Table 2. Inputs given for the ANN models [4, 35-37]

BD	12:0	14:0	16:0	16:1	18:0	18:1	18:2	18:3	20:1	22:1	CN
lauric	100	0	0	0	0	0	0	0	0	0	61.4
myristic	0	100	0	0	0	0	0	0	0	0	66.2
palmitic	0	0	100	0	0	0	0	0	0	0	74.5
stearic	0	0	0	0	100	0	0	0	0	0	86.9
oleic	0	0	0	0	0	100	0	0	0	0	55.0
palmitoleic	0	0	0	100	0	0	0	0	0	0	51.0
linoleic	0	0	0	0	0	0	100	0	0	0	42.2
erucic	0	0	0	0	0	0	0	0	0	100	76.0
eicosanoic	0	0	0	0	0	0	0	0	100	0	64.8
linolenic	0	0	0	0	0	0	0	100	0	0	20.4
soybean	0	0.1	10.5	0.1	3.7	23.2	48.9	1.2	0.3	0.1	47.2
inedible tallow	0.1	2.1	23.9	2.8	19.5	38.5	6.4	0.3	0.5	0.1	61.7
Thevetia peruviana M.	0	0	15.6	0	10.5	60.9	5.2	7.4	0	0	57.5
Moringa oleifera Lam	0	0	9.1	2.1	2.7	79.4	0.7	0.2	0	0	56.7
Pongamia pinnata P.	0	0	10.6	0	6.8	49.4	19.0	0	2.4	0	55.8
Holoptelia integrifolia	0	3.5	35.1	1.9	4.5	53.3	0	0	0	0	61.2
Vallaris solanacea K.	0	0	7.2	0	14.4	35.3	40.4	0	0	0	50.3
Aleurites moluccana	0	0	5.5	0	6.7	10.5	48.5	28.5	0	0	34.2
Euphorbia helioscopia L	2.8	5.5	9.9	0	1.1	15.8	22.1	42.7	0	0	34.2
Garnicia morella D.	0	0	0.7	0	46.4	49.5	0.9	0	0	0	63.5
Saturega hortensis Linn	0	0	0.4	0	0.4	12.0	18.0	62.0	0	0	25.5
Actinodaphne angust.	87.9	1.9	0.5	0	5.4	0	0	0	0	0	63.2
Litsea glutinosa Robins	96.3	0	0	0	0	2.3	0	0	0	0	64.8
Neolitsea cassia Linn	85.9	3.8	0	0	0	4.0	3.3	0	0	0	64.0
Swietenia mahagoni J.	0	0	9.5	0	18.4	56.0	0	16.1	0	0	52.3

Table 2. (a) Inputs given for the ANN models [34, 35, 37, 38]

BD	12:0	14:0	16:0	16:1	18:0	18:1	18:2	18:3	20:1	22:1	CN
Argemone mexicana	0	0.8	14.5	0	3.8	18.5	61.4	0	0	0	44.5
Salvadora persica Linn	19.6	54.5	19.6	0	0	5.4	0	0	0	0	67.5
Madhuca butyracea M.	0	0	66.0	0	3.5	27.5	3.0	0	0	0	65.3
Rhus succedanea Linn	0	0	25.4	0	0	46.8	27.8	0	0	0	52.2
Basella rubra Linn	0	0.4	19.7	0.4	6.5	50.3	21.6	1.1	0	0	54.0
Corylus avellana	0	3.2	3.1	0	2.6	88.0	2.9	0	0	0	54.5
Jatropa curcas Linn	0	1.4	15.6	0	9.7	40.8	32.1	0	0	0	52.3
Croton tiglium Linn	0	11.0	1.2	0	0.5	56.0	29.0	0	0	0	49.9
Princeptia utilis Royle	0	1.8	15.2	0	4.5	32.6	43.6	0	0	0	48.9
Vernonia cinerea Less	0	8.0	23.0	0	8.0	32.0	22.0	0	0	0	57.5
Joannesia princeps V.	0	2.4	5.4	0	0	45.8	46.4	0	0	0	45.2
Garcinia combogia D.	0	0	2.3	0	38.3	57.9	0.8	0.4	0.3	0	61.5
Garcinia indica Choisy	0	0	2.5	0	56.4	39.4	1.7	0	0	0	65.2
Illicium verum Hook	0	4.4	0	0	7.9	63.2	24.4	0	0	0	50.7
Melia azadirach Linn	0	0.1	8.1	1.5	1.2	20.8	67.7	0	0	0	41.4
Myristica malabarica L	0	39.2	13.3	0	2.4	44.1	1.0	0	0	0	61.8
Urtica dioica Linn	0	0	9.0	0	0	14.6	73.7	2.7	0	0	38.7
Tectona grandis Linn	0	0.2	11.0	0	10.2	29.5	46.4	0.4	0	0	48.3
canola	0	0.1	5.2	0.2	2.5	58.1	28.1	0.4	1.6	0.4	55.0
lard	0.1	1.9	24.5	2.8	14.4	38.3	13.4	0.3	0.7	0.1	63.6
yellow grease	0	1.1	17.3	2.2	9.5	45.3	14.5	1.3	1.3	0	52.9
rape	0	0	4.8	0	1.6	33.0	20.4	7.9	9.3	23.0	55.0
linseed	0	0	5.0	0	2.0	20.0	18.0	55.0	0	0	52.0

3. Results and Discussion

The search for the optimal network for predicting the CN was based in the absolute error as the objective function in the processes, but combining it with adequate values of the correlation coefficients. The results from the whole ANNs in order find better CN prediction capabilities based on the FAME as input parameters are shown in Table 2 and Table 3.

The results shown in Table 3 are corresponding to the trained ANNs changing the phase two among six algorithms, varying the nodes number between 3 and 7 and using the linear as output function. The Table 4 shows the results for the same method but corresponding to a logistic output function.

Table 3. Absolute errors and correlation coefficients of cetane number estimation using a linear output function

nodes	BP	CGD	DBD	LM	QN	QP
3	2.7 (92.5)	2.4 (93.5)	2.4 (94.9)	1.9 (94.6)	1.9 (94.5)	2.0 (95.9)
4	2.9 (93.4)	1.6 (96.3)	2.3 (94.3)	2.3 (93.0)	1.5 (95.7)	2.4 (94.6)
5	2.3 (93.9)	2.6 (94.9)	2.0 (95.3)	2.3 (95.2)	2.1 (95.9)	2.1 (95.0)
6	2.3 (92.7)	2.5 (94.3)	2.0 (93.5)	1.9 (94.9)	2.4 (92.4)	1.9 (95.7)
7	2.7 (94.0)	2.3 (94.9)	2.6 (92.6)	2.0 (95.8)	1.8 (95.4)	2.1 (94.3)

Both tables have shown the absolute errors and the coefficients of correlation (in parenthesis). The correlation coefficients were in all cases higher than 91%. The critical point is that in many cases it is not possible to obtain absolute error values below 2, as is observed in Table 3 and Table 4. Only eight ANNs are below this value.

Basu [31] also reported the use of 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 coefficients higher than 95% for the network in the training step. Yang [12] obtained 2.1 of mean absolute error for a three layer backpropagation network but his network is only applied to diesel fuels. Ramadhas [15] used four types of ANN, 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 numbers between 22.7-75.6, similar to the range applied in the present work.

Three ANN were selected for the validation step, two of them according to the lowest absolute errors combined with two of the highest correlation coefficients found. The third one is an ANN previously published by the authors of this paper [9] that is also included in Table 3, in order to compare with the better proposal among 24 ANN tested, and previously published.
The first two ANNs selected were corresponding to the use of a linear output function in the network and four nodes in the hidden layer. As can be observed in Table 3, the lowest absolute error values were obtained for CGD and GN algorithms. Therefore, both were selected for the validation step. The third one is corresponding to the LM algorithm with 5 nodes and a linear output function.

Table 4. Absolute errors and correlation coefficient of cetane number estimation using a logistic output function

nodes	BP	CGD	DBD	LM	QN	QP
3	2.2 (94.0)	2.1 (94.4)	2.6 (91.4)	2.2 (95.4)	2.4 (94.2)	2.3 (93.3)
4	2.8 (93.0)	2.7 (92.8)	2.4 (92.9)	2.3 (94.8)	2.5 (94.7)	2.4 (94.2)
5	2.2 (93.3)	2.5 (94.8)	2.0 (92.9)	2.4 (93.8)	2.2 (95.7)	2.1 (96.1)
6	2.1 (92.4)	2.3 (94.2)	2.0 (93.3)	2.7 (93.3)	2.0 (94.3)	2.4 (92.6)
7	1.9 (94.8)	2.3 (93.5)	2.2 (91.1)	2.5 (91.0)	2.5 (93.1)	2.3 (91.0)

Models validation

For the validation of the models selected, a data set not related to the modeling data (Table 2) was used. The validation data covers 15 samples from other references. The collected data includes the experimental evaluation of FAME composition and CN, covering a wide range of possible values of cetane number (between 41 and 69) and they were taken from experiments using engine tests or an ignition quality tester. All the information about the validation data is presented in Table 5. All

the values in Table 5 are in weight percentage. The prediction capability of the selected models for this external data were based in the comparison between the predicted cetane number by the ANN and the experimental value (actual value) trying to find less residuals for the whole tested data. A compendium of the main results of the validation process for the three selected models is shown in Table 6. The analysis of the models shown that the prediction capability of the model that uses the CGD is better than using the QN algorithm.

In a less extensive previous work [9], the authors of this work proposed as the best model a LM (11:5:1) with linear output function among 24 ANN, because it showed the best prediction capability for the validation data. But it this work, as is observed in Table 3, several ANN suggest better performance than the previously published, therefore it won't be taken into account for the validation process.

Table 5. Experimental data selected for models validation [34, 35, 38, 41-43]

sample	12:0	14:0	16:0	16:1	18:0	18:1	18:2	18:3	20:1	22:1	CN
wild mustard	0	0.1	2.6	0.2	0.9	7.8	14.2	13.0	5.4	45.7	61.1
waste palm oil	0	1.0	39.0	0.2	4.3	43.7	10.5	0.2	0.2	0	60.4
Balanites roxburhii	0	0	17.0	4.3	7.8	32.4	31.3	7.2	0	0	50.5
Garnicia echinocarpa	0	0	3.7	0	43.7	52.6	0	0	0	0	63.1
Neolitsea umbrosa G.	59.1	11.5	0	0	0	21.0	6.7	0	0	0	60.8
Anamirta cocculus	0	0	6.1	0	47.5	46.4	0	0	0	0	64.3
Broussonetia p.Vent.	0	0	4.0	0	6.1	14.8	71.0	1.0	0	0	41.2
Salvadora oleoiles D.	35.6	50.7	4.5	0	0	8.3	0.1	0	0	0	66.1
Nephelium L.	0	0	0.2	0	13.8	45.3	0	0	4.2	0	64.9
Ziziphus maurit. L.	0	0	10.4	0	5.5	64.4	12.4	0	2.6	1.7	55.4
jojoba	0	0	1.2	0	0	10.7	0.1	0.4	59.5	12.3	69.0
rape	0	0	4.9	0	1.6	33.0	20.4	7.8	9.3	23.0	55.0
peanut	0	0.1	8.0	0	1.8	53.3	28.4	0.3	2.4	0	53.0
grape	0	0.1	6.9	0.1	4.0	19.0	69.1	0.3	0	0	48.0
sunflower	0	0	6.0	0.1	2.9	17.0	74.0	0	0	0	49.0

As is shown in Fig.1, in many evaluated points, the prediction is better using the ANN (11:4:1) with CGD 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 with a total sum of 150 for 190 using the QN algorithm.

In the comparison between both models shown in Fig.1, even when there are some points with the same predicted values for both, a general analysis of outlier points shows that the best algorithm for CN prediction is the CGD. The zone in Fig.1 that covers the range 50-62 of cetane number corresponds to the common CN value of biodiesel from many feedstocks. As is observed, this is the zone that shows the lowest outlier points in both cases.

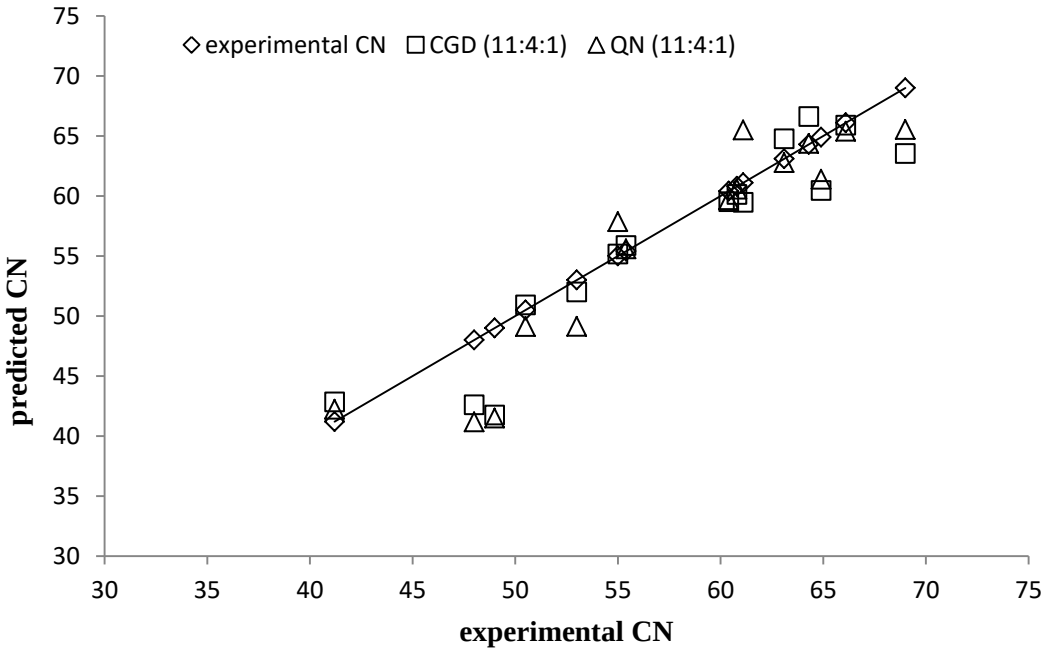

Fig.1 Comparison between selected ANNs for prediction of CN corresponding to the validation data

Ramadhas [15] reported accuracy between 3.4-5.0% for predicting the CN, depending of the type of neural network used for the CN prediction, but he used only 5 FAMEs as inputs, therefore the prediction capability of his 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. The main statistical results of the validation process are shown in Table 6. There can be observed that mainly based in the sum of squares for the residuals and the correlation coefficient obtained, the more adequate ANN is the based on CGD algorithm.

Table 6. Main statistical results for the models selected in the validation process

ANN	Absolute Error	*R* for the validation data	Sum of squares for the residuals
CGD (11:4:1)	1.6	93.8%	150.3
QN (11:4:1)	1.5	93.7%	196.0

Therefore, the best network is the implemented using a topology (11:4:1) of 11 inputs, 1 output variable and four nodes. This ANN was implemented using two phases in the training step (backpropagation and Conjugate Gradient Descend). The response surface obtained for this CGD

(11:5:1) network for the prediction of the CN as function of Myristic and Lauric is shown in Fig.2. This was the only two dimensional relationship obtained with a change in the influence in the CN depending of the value of the factor, in this case, the Palmitoleic percentage.

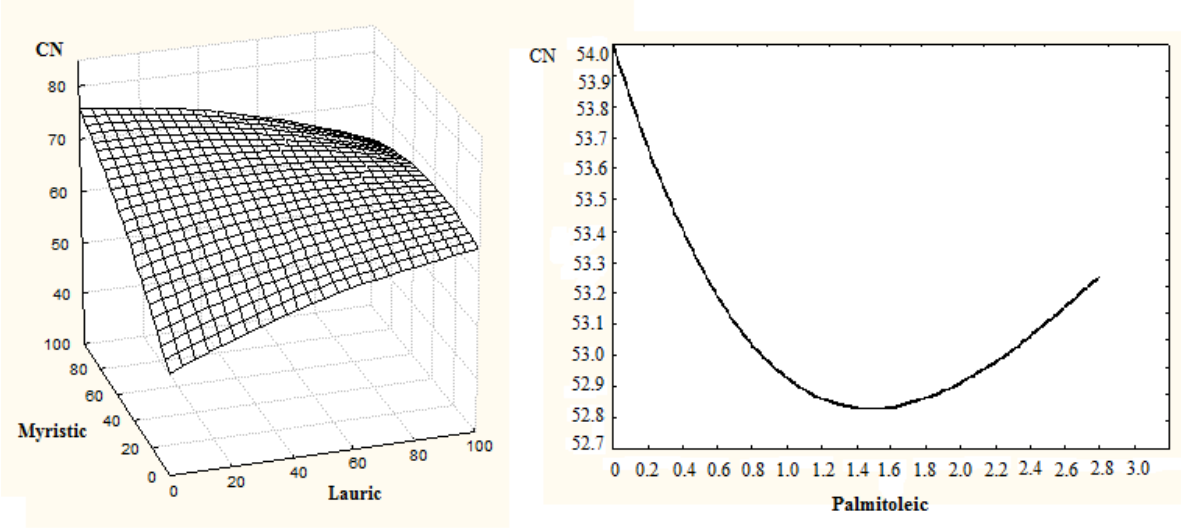

Fig.2 Response surface and dependence of Palmitoleic percentage for CN using a CGD (11:4:1)

Using the results of the validation process, the percentage of accuracy in the prediction was evaluated, referring to the actual or experimental values of cetane number. Lack of accuracy was observed in certain cases of the validation when the total percentage of unsaturation in the FAME composition of the biodiesel. As is observed in Fig.3, beyond a value corresponding to near 80% of total unsaturation, in some cases the uncertainty percent are increased, reaching values higher than 5%.

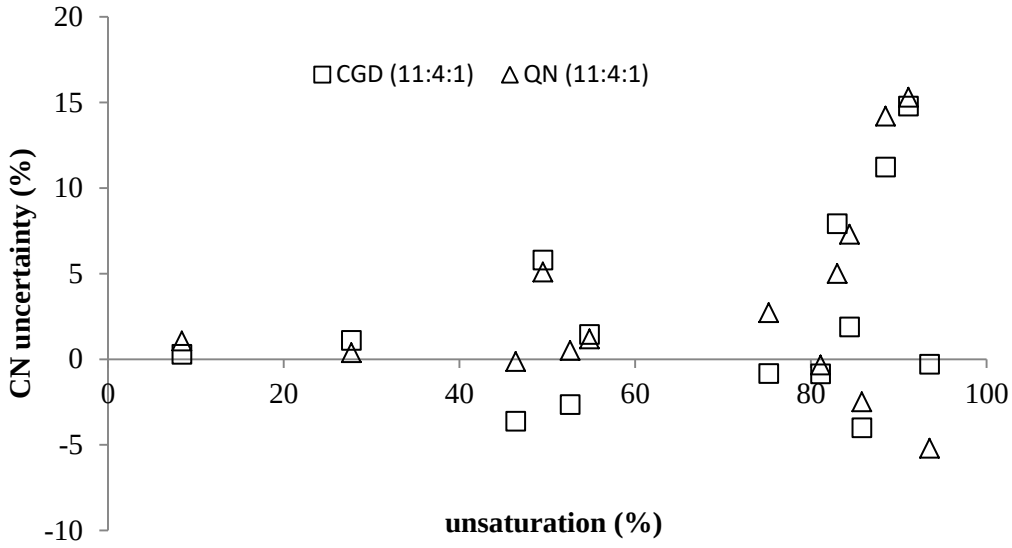

Fig.3 Dependence of the uncertainties percent with the percent of unsaturation for the selected ANN

According to Fig.3, even when some values are well predicted by one or both ANN, the general behavior is to lower accuracies when the unsaturation percent is higher than 80%, therefore the selected best model can fail in this critical range of total unsaturation. Therefore, we recommend the use of the selected and validated model for the prediction of CN only in a range of total unsaturation in the biodiesel lower than 80%. In the proposed 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 FAME different that the selected for this work.

4. Conclusions

A model to predict the cetane number based on the composition of ten FAME presented in biodiesel using an artificial neural network was obtained with better accuracy than 95%. 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 and showing 93.8% of correlation for the validation data and a mean absolute error of 1.5. The proposed network is useful for prediction of the cetane number of biodiesel in a wide range of FAME composition but keeping the percentage of total unsaturation lower than 80%.

References

1. Yuan, W., A.C. Hansen, and Q. Zhang, *Vapor pressure and normal boiling point predictions for pure methyl esters and biodiesel fuels.* Fuel, 2005. **84**: p. 943-950.
2. Wadumesthrige, K., et al., *Investigation of the Parameters Affecting the Cetane Number of Biodiesel.* J Am Oil Chem Soc, 2008. **85**: p. 1073-1081.
3. Ramirez-Verduzco, L.F., J.E. Rodriguez-Rodriguez, and A. Jaramillo-Jacob, *Predicting cetane number, kinematic viscosity, density and higher heating value of biodiesel from its fatty acid methyl ester composition.* Fuel, 2012. **91**: p. 102-111.
4. Knothe, G., *Dependence of biodiesel fuel properties on the structure of fatty acid alkyl esters.* Fuel Processing Technology, 2005. **86**: p. 1059-1070.
5. Knothe, G., *Cetane numbers of branched and straight-chain fatty esters determined in an ignition quality tester.* Fuel, 2003. **82**(8): p. 971-975.
6. Icingur, Y. and D. Altiparmak, *Effect of fuel cetane number and injection pressure on a DI Diesel engine performance and emissions.* Energy Conversion & Management, 2003. **44**(3): p. 389-397.
7. Piloto-Rodriguez, R., R. Sierens, and S. Verhelst, *Ignition delay in a palm oil and rapeseed oil biodiesel fuelled engine and predictive correlations for the ignition delay period.* Fuel, 2011. **90**: p. 766-772.
8. Sanchez-Borroto, Y., et al., *Predicción del número de cetano de biocombustibles a partir de su composición de ácidos grasos.* Ingeniería Mecánica, 2012. **15**(2): p. 147-157.
9. Piloto, R., et al., *Prediction of the cetane number of biodiesel using artificial neural networks and multiple linear regression.* Energy Conversion & Management, 2013. **65**: p. 255-261.
10. Van Gerpen, J.H. *Cetane number testing of biodiesel*. in *Proceedings of the Third Liquid Fuel Conference. Liquid fuels and industrial products from renewable resources*. 1996. Nashville.
11. Murphy, M.J., J.D. Taylor, and R.L. McCormick, *Compendium of experimental cetane number data*, N.R.E. Laboratory, Editor 2004, National Renewable Energy Laboratory: Colorado.
12. Yang, H., et al., *Neural network prediction of cetane number and density of diesel fuel from its chemical composition determined by LC and GC-MS.* Fuel, 2002. **81**: p. 65-74.
13. Gopinath, A., S. Puhan, and G. Nagarajan, *Relating the cetane number of biodiesel fuels to their fatty acid composition: a critical study.* Journal of Automobile Engineering, 2009. **223**: p. 565-583.
14. Krisnangkura, K., *A simple method for estimation of cetane index of vegetable oil methyl esters.* J. Am. Oil Chemists' Soc., 1980. **63**(4): p. 552-553.

15. Ramadhas, A.S., et al., *Artificial neural networks used for the prediction of the cetane number of biodiesel fuel.* Renewable Energy, 2006. **31**: p. 2524-2533.
16. Lapuerta, M., J. Rodriguez-Fernandez, and O. Armas, *Correlation for the estimation of the density of fatty acid esters fuels and its implications. A proposed Biodiesel Cetane Index.* Chemistry and Physics of Lipids 2010. **163**: p. 720-727.
17. Lapuerta, M., J. Rodriguez-Fernandez, and E. Font de Mora, *Correlation for the estimation of the cetane number of biodiesel fuels and implications on the iodine number.* Energy Policy, 2009. **37**: p. 4337-4344.
18. Bamgboye, A.I. and A.C. Hansen, *Prediction of cetane number of biodiesel fuel from the fatty acid methyl ester (FAME) composition.* Int. Agrophysics, 2008. **22**: p. 21-29.
19. Esen, H., et al., *Performance prediction of a ground-coupled heat pump system using artificial neural networks.* Expert Systems with Applications, 2008. **35**(4): p. 1940-1948.
20. Esen, H., et al., *Forecasting of a ground-coupled heat pump performance using neural networks with statistical data weighting pre-processing.* Int. J. of Thermal Sciences, 2008. **47**(4): p. 431-441.
21. Esen, H., et al., *Modeling a ground-coupled heat pump system by a support vector machine.* Renewable Energy, 2008. **33**(8): p. 1814-1823.
22. Esen, H., et al., *Modeling of a new solar air heater through least-squares support vector machines.* Expert Systems with Applications, 2009. **36**(7): p. 10673-10682.
23. Karatepe, E., M. Boztepe, and M. Colak, *Neural network based solar cell model.* Energy Conversion & Management, 2006. **47**(9-10): p. 1159-1178.
24. Kalogirou, S.A., *Application of artificial neural networks in energy systems. A review.* Energy Conversion & Management, 1999. **40**(10): p. 1073-1087.
25. In-Ho, Y., Y. Myoung-Souk, and K. Kwang-Woo, *Application of artificial neural network to predict the optimal start time for heating system in building.* Energy Conversion & Management, 2003. **44**(17): p. 2791-2809.
26. Reddy, K.S. and M. Ranjan, *Solar resource estimation using artificial neural networks and comparison with other correlation models.* Energy Conversion & Management, 2003. **44**(15): p. 2519-2530.
27. Kalogirou, S.A., *Artificial intelligence for the modeling and control of combustion processes: a review.* Progress in Energy and Combustion Science, 2003. **29**: p. 515-566.
28. Blasco, J.A., et al., *A self organizing- map approach to chemistry representation in combustion applications.* Combust Theory Modeling, 2000. **4**(1): p. 61-76.
29. Heister, F. and M. Froehlich, *Non-linear time series analysis of combustion pressure data for neural network training with the concept of mutual information.* Proc Inst Mech Engnr, Part D: J Automobile Engng, 2001. **215**(D2): p. 299-304.
30. Thompson, G.J., et al., *Neural network modeling of the emissions and performance of a heavy-duty diesel engine.* Proc Inst Mech Engnr, Part D: J Automobile Engng, 2001. **214**(D2): p. 111-126.
31. Basu, B., et al., *A Neural Network Approach to the Prediction of Cetane Number of Diesel Fuels Using Nuclear Magnetic Resonance (NMR) Spectroscopy.* Energy & Fuels, 2003. **17**: p. 1570-1575.
32. Santana, R.C., et al., *Evaluation of different reaction strategies for the improvement of cetane number in diesel fuels.* Fuel, 2006. **85**: p. 643-656.
33. Korres, D.M., et al., *A neural network approach to the prediction of diesel fuel lubricity.* Fuel, 2002. **81**: p. 1243-1250.
34. Ramos, M.J., et al., *Influence of fatty acid composition of raw materials on biodiesel properties.* Bioresource Technology, 2009. **100**: p. 261-268.
35. Mohibbe, A.M., A. Waris, and N.M. Nahar, *Prospects and potential of fatty acid methyl esters of some non-traditional seed oils for use as biodiesel in India.* Biomass & Bioenergy, 2005. **29**: p. 293-302.

36. Tong, D., et al., *Cetane Number Prediction of Biodiesel from the Composition of the Fatty Acid Methyl Esters.* J Am Oil Chem Soc, 2011. **88**: p. 415-423.
37. Kinast, J.A., *Production of Biodiesels from Multiple Feedstocks and Properties of Biodiesels and Biodiesel/Diesel Blends*, in *NREL/SR-510-31460*, NREL, Editor 2003, NREL: Illinois.
38. Agarwal, A.K., *Biofuels (alcohols and biodiesel) applications as fuels for Internal Combustion Engines.* Progress in Energy and Combustion Science, 2007. **33**: p. 233-271.
39. Moser, B.R., *Biodiesel production, properties, and feedstocks.* In Vitro Cell. Dev. Biol. Plant, 2009. **45**: p. 229-266.
40. Huajin, T., T. Kay Chen, and Y. Zhang, *Neural Networks: Computational Models and Applications*. Studies in Computational Intelligence. Vol. 53. 2007, Berlin: Springer. 288.
41. Ozsezen, A.N. and M. Canakci, *Determination of performance and combustion characteristics of a diesel engine fueled with canola and waste palm oil methyl esters.* Energy Conversion and Management, 2011. **52**: p. 108-116.
42. Jham, G.N., et al., *Wild Brazilian Mustard (Brassica juncea L.) Seed Oil Methyl Esters as Biodiesel Fuel.* J Am Oil Chem Soc, 2009. **86**: p. 917-926.
43. Shah, S.N., et al., *Preparation and Evaluation of Jojoba Oil Methyl Esters as Biodiesel and as a Blend Component in Ultra-Low Sulfur Diesel Fuel.* Bioenergy Resources, 2010. **3**: p. 214-223.