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Full Length Article

# Improved estimation of Cetane number of fatty acid methyl esters (FAMEs) based biodiesels using TLBO-NN and PSO-NN models

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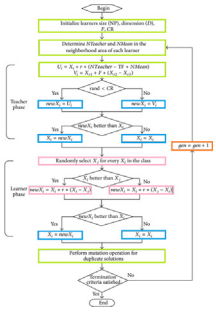
## GRAPHICAL ABSTRACT



## ARTICLE INFO

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## ABSTRACT

Cetane number (CN) is one of the key factors of biodiesels and other diesel fuels. It is an indicator of ignition speed and required compression for ignition. CN estimation of biodiesel based on fatty acid methyl esters (FAME) composition was the main goal of this work. Application of artificial neural network (ANN) combined with particle swarm optimization (PSO) and teaching-learning based optimization (TLBO) is discussed in this communication. A number of 232 fuel samples was derived from the literature as the raw data for the models development. Different evaluative factors prove the satisfactory performance of the proposed ANN models. The obtained values of R-squared and mean square of errors are 0.973 & 3.538 and 0.951 & 6.324 for the proposed TLBO-ANN and PSO-ANN, respectively. Based on the outcome of this study, ANN coupled with PSO and TLBO algorithms can be suitable tools, especially TLBO algorithm to estimate CN of biodiesels.

## 1. Introduction

Issues such as global warming, the completion of fossil fuels, environmental preservation, etc have been stimuli to take steps to achieve clean and renewable energies. Biodiesel is one of the renewable and biodegradable sources of energy [1–4], being produced typically via transesterification which is a chemical reaction between vegetable oils or animal fats with alcohols such as methanol or ethanol in the presence of alkaline catalysts. Different types of fatty acid methyl esters (FAME) exist in the biodiesel composition with different carbon chain lengths, molar mass, fatty acid methyl ester mass ratio, and carbon-carbon binary bonds which in turn affect biodiesel specifications [5,6]. ASTM

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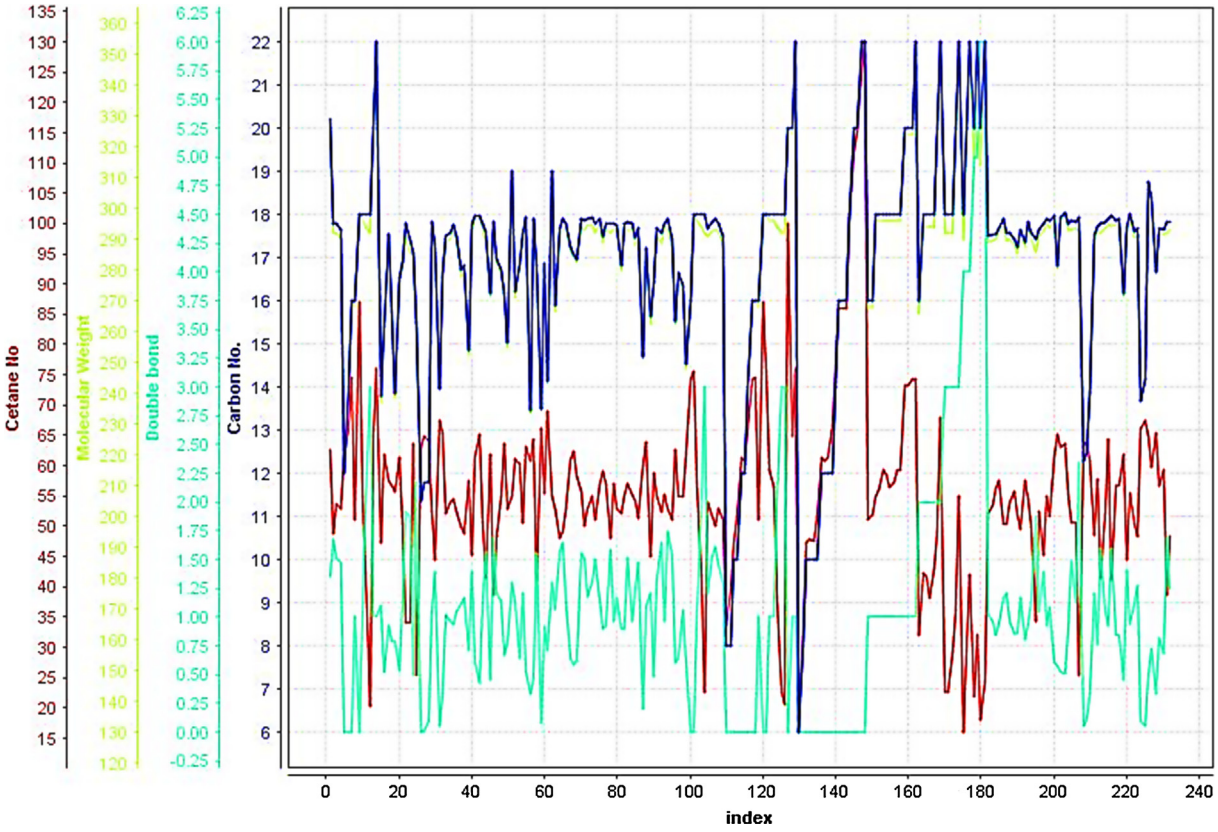


**Fig. 1.** Ranges of experimental data used for developing the models.

D6751 and EN 14,214 (based on previous DIN 51606) are widely used to specify the biodiesel characteristics [7]. One of the key factors of biodiesel is Cetane number (CN), an indicator of ignition speed and required compression for ignition. Combustion behavior, engine power, and pollutant emissions are highly affected by Cetane number [8].

Cooperative fuel research (CFR) engine method (ASTM D613), fuel ignition tester (FIT) method (ASTM D7170), ignition quality tester (IQT) method (ASTM D6890), and Cetane index (CI) method (ASTM D4737 or ASTM D976) have been developed to determine Cetane number [2,9–13]. All of the methods are difficult and expensive [14–16], for instance, the method introduced in ASTM D613, about measuring the Cetane number includes mixing reference fuels (*n*-Cetane and hepta-methylnonane) in different volumetric compositions under a defined test condition [17]. Obtaining such conditions and materials may not be always simple. As a result, one of the most interesting options is an estimation of the fuel quality characteristics based on its physicochemical and structural specifications. Recently, application of artificial intelligence such as artificial neural network has been increased in chemical and petroleum engineering due to its satisfactory results [18–21].

Miraboutalebi et al. developed and compared the random forest (RF) and ANN models to estimate CN based on the fatty acid methyl esters content of biodiesel [15]. According to $R^2$ and Root Mean Squared Error (RMSE), ANN ($R^2$ = 0.95, RMSE = 2.53) shows to be superior to RF ($R^2$ = 0.92, RMSE = 3.09), however, RF could be more easily and widely applied in CN determination. They indicated that in such a way that among fatty acid methyl ester, unsaturated linoleic acid has the most significant effect on Cetane number prediction. Multiple linear regression model (MLRM) was used to correlate CN and fatty acid methyl ester (FAME) of biodiesel by Tong et al. [22]. The proposed regression equation has a very good coefficient of determination ($R^2$ = 0.9904) and acceptable accuracy (average absolute error of 1.52 for all data). The application of multiple linear regression has an accuracy of 89% while artificial neural networks (ANN) provided a slightly higher accuracy of 92% [23]. Partial least square (PLS) based on ANN was also used to estimate CN from its FAMEs by Hosseinpour et al. [14]. Furthermore, they compared the performance of PLS adapted by ANN with classical PLS. They demonstrated that there is an increase of $R^2$ = 0.85 of classical PLS to more than 0.99 in PLS adapted by ANN. In another study, the effect of biodiesel composition on Cetane number was defined through straight-chain saturated factor (SCSF) and modified the degree of unsaturation ($DU_m$) comparing 9 different biodiesel fuels [17]. The regression coefficient of 0.95 and average absolute deviation of 1.63 was reported in this study.

Using artificial neural network method to obtain CN from its FAMEs profile was the main goal of this work. The performance of the developed models is compared by multiple statistical criteria such as $R^2$, RMSE, STD, and MAPE. These criteria may be close to each other and may not have a uniform trend. Therefore, individual and overall desirability functions are defined for the mentioned criteria.

## 2. Theory

### 2.1. Multi-layer perceptron artificial neural network (MLP-ANN)

ANN algorithm is mainly based on input layer hidden layer(s) and output layer [24–26]. Layers are based on some nodes which are inspired by neurons and there are linked connections between these nodes. A weighted parallel linking formation is responsible for the connections. Self-organizing map, multi-layer perceptron, multilayer recurrent, and cellular neural networks are some commonly applied ANN algorithms. The multi-layer artificial neural network is more favored in the literature.

ANN most important parts are the bias and the weight. During initialization degree of freedom is defined by the bias values, moreover, weight values control the linked connections between the nodes