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Application of artificial neural networks to predict viscosity, iodine value and induction period of biodiesel focused on the study of oxidative stability

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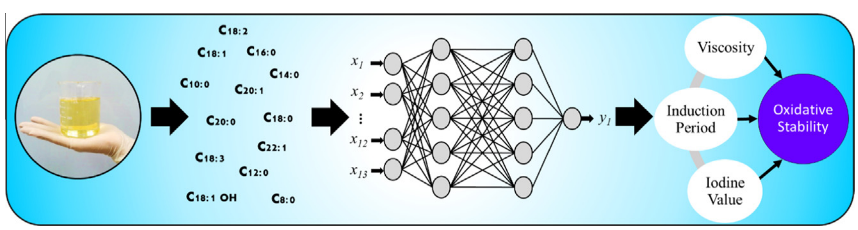
HIGHLIGHTS

- Good performance of a model of ANN to predict quality parameters of biodiesel.
- Quality of biodiesel.
- Useful tool to evaluate the potential of raw materials to produce biodiesel.

GRAPHICAL ABSTRACT

ANN has been applied on prediction of viscosity, iodine value and induction period of biodiesel, whose properties directly reflect its level of degradation, to evaluate the oxidative stability. The method indicates be useful as a tool to evaluate the potential of raw materials to produce a biodiesel with good oxidative stability and to reach improvements concerning official methods.



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ABSTRACT

In the search for alternative fuels that can gradually replace petroleum derivatives, biodiesel is highlighted as a substitute for diesel and it is defined as a biofuel obtained from transesterification of triglycerides. Despite of several advantages over mineral diesel, an elementary disadvantage of biodiesel is its low oxidative stability, which is strongly influenced by the unsaturation degree of its fatty acid methyl esters (FAMEs) and by the conditions to which biodiesel is exposed during storage, transporting and handling. The present work focuses on the optimization and application of artificial neural networks (ANNs) on prediction of viscosity, iodine value and induction period of biodiesel, properties that directly reflect its level of degradation, to evaluate the oxidative stability. The input variables were the percentages of the 13 most common FAMEs in biodiesels and the transesterification does not change the fatty esters profile of the raw material. In this case the ANN method allows predicting viscosity, iodine value and induction period, either before transesterification, after synthesis of biodiesel or during the storage. Therefore, this method can be useful as a tool to evaluate the potential of raw materials to produce a biodiesel with good oxidative stability and to reach improvements concerning official methods. The optimization process of the ANN occurred in three steps: test of algorithms for adjusting weights, test of stopping condition and test of activation functions, and the physicochemical properties were treated independently. For

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the set of test samples, which simulates real samples, the application of the optimized ANNs provided results with root mean squared errors (RMSE) of 0.55 mm^2/s, 3.49 g/100 g and 0.89 h for viscosity, iodine value and induction period, respectively, what ensures the feasibility of the proposed method. A comparison between the proposed method and linear methods from literature, both based on the biodiesel composition indicates that our ANN model is much more adequate to the problem addressed.

1. Introduction

In the last few years, the search for alternative fuels that can gradually replace petroleum derivatives has been motivated mainly for energetic security reasons and environmental factors [1]. In this context, biodiesel is highlighted as an alternative for using mineral diesel, and it is defined as a mixture of linear chain alkyl esters, obtained from transesterification of triglycerides of oils and fats with short chain alcohols.

Despite of biodiesel presents better lubricity and biodegradability, lower toxicity, essentially no sulfur content and higher flash point, as well as other advantages over mineral diesel, an elementary disadvantage of biodiesel is its low oxidative stability [2,3], characteristic that becomes very important considering that biodiesel can take months after its production until it reaches the final consumer. The conditions to which biodiesel is exposed during storage, transporting and handling, as high temperatures, contact with metallic surfaces, presence of air, light or impurities, can accelerate its degradation, influencing its composition and, thereafter, its quality [3].

The main products formed by oxidation of biodiesel are aldehydes, ketones, peroxides, epoxides, alcohols and short chain carboxylic acids [4], which can form insoluble gums and cause filter clogging, injector coking and corrosion of engine metallic parts [5,6]. These damages make of oxidative stability an evidently important characteristic for biodiesel quality during storage period, and to study it, should be considered some parameters as viscosity, iodine value and, above all, induction period, which directly reflect the level of biodiesel degradation.

Kinematic viscosity measures the flow resistance of a fluid and it increases with size of the carbonic chains and with unsaturation degree [7,8], as well as with the presence of products of biodiesel oxidation, since the degradation leads to formation of saturated products and free fatty acids, which have higher viscosity than its corresponding esters [4]. High viscosity causes decrease in injection flow and atomization, incomplete combustion and consequently, formation of deposits in combustion chamber [8,9].

Iodine value quantifies the unsaturations of the esters present in the biodiesel and it is determined by the quantity of grams of iodine that reacts directly with double or triple bonds between carbon atoms, for each 100 g of biodiesel [7,10]. A high unsaturation degree leads to decrease of cetane number and of oxidative stability of the biofuel. Over time, the decrease of iodine value of a sample evinces the increase of oxidative degradation [11], which allows monitoring the biodiesel deterioration.

Induction period is the most important parameter related to oxidative stability of biodiesel, because it estimates for how long the sample will resist to degradation by oxidation [3]. The test is based on the increase of conductivity of deionized water in a vessel that retains volatile products formed during the accelerated oxidation of biodiesel at 110 °C [2,12]. The more unsaturated the esters of biodiesel, the greater its tendency to oxidate and the shorter the induction period [4,6].

Viscosity and iodine value, besides other physicochemical properties, presented a good correlation with unsaturation degree of esters, in a work developed by Hoekman and collaborators, involving the study of the composition of 221 samples of biodiesel [7]. We also can mention the development of an equation, in studies of Park et al., that correlates the amount of linoleic and linolenic acids to the induction period, in mixtures of biodiesels of palm, rapeseed and soybean [13]. Many other studies also show the influence of composition in some properties of biodiesel [4,14–18].

Due to the strong relation between the composition of biodiesel and its viscosity, iodine value and induction period, the present work aims to apply ANN on the prediction of these properties focusing on the study of oxidative stability of biodiesel, from the mass percentages of FAMEs present in the samples.

Since the transesterification does not change the fatty esters profile of the raw material [7,14], the application of neural networks allows to predict the three mentioned properties, either before transesterification (from composition of the oil or fat) after synthesis of biodiesel or during the storage. This enables to monitor oxidative stability at any time since selection of the raw material until distribution or consumption of the biofuel.

Some of the official methods to certify the quality of biodiesel can require equipments of high costs of acquisition, operation and maintenance, besides being relatively complex or even time consuming, such as the methods to determine viscosity, iodine value and induction period. Thus, it becomes extremely relevant the estimation of the quality parameters of biodiesel, even before its transesterification, to evaluate the potential of vegetal raw materials to produce a biodiesel with good oxidative stability and to reach improvements concerning official methods.

2. Database preparation

A database containing the chemical composition and three physicochemical parameters (viscosity, iodine value and induction period) of biodiesel samples was elaborated with two kinds of experimental data (one was ceded by the Laboratory of Analysis and Research on Petroleum Analytical Chemistry (LAPQAP/UFMA) and the other one was from literature data [2,7,11,13,19–27]).

The compositions of all 98 samples comprise 13 methyl esters of the following fatty acids: caprylic acid (C8:0), capric acid (C10:0), lauric acid (C12:0), myristic acid (C14:0), palmitic acid (C16:0), stearic acid (C18:0), oleic acid (C18:1), linoleic acid (C18:2), linolenic acid (C18:3), arachidic acid (C20:0), gadoleic acid

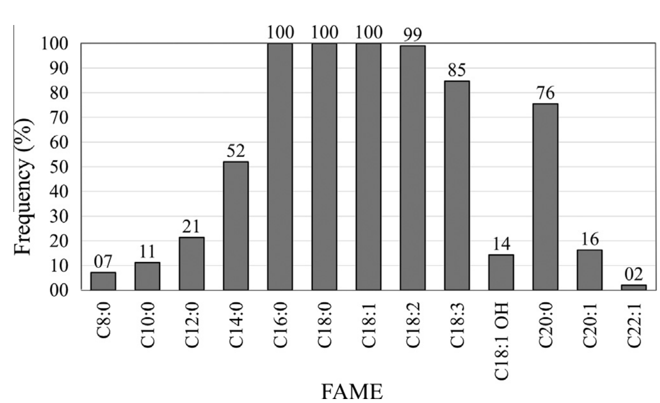

Fig. 1. Histogram of the presence of each fatty acid ester in the samples of biodiesel.