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Full Length Article

Prediction capabilities of mathematical models in producing a renewable fuel from waste cooking oil for sustainable energy and clean environment

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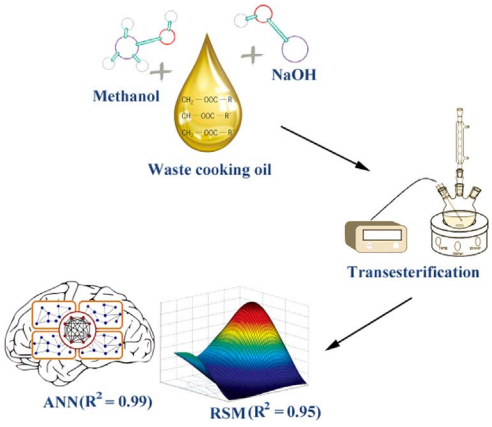
GRAPHICAL ABSTRACT



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ABSTRACT

The present work describes the comparison of biodiesel yield prediction by Response Surface Methodology (RSM) and Artificial Neural Network (ANN). The prediction models were developed based on three-level design of experiments conducted with waste cooking oil transesterified by varying four process parameters such as catalyst concentration, molar ratio, reaction time, and stirrer speed. The optimum reaction conditions were found to be 0.75% wt/wt catalyst concentration, 9:1 M ratio, 60 min reaction time and 500 rpm stirrer speed. For these optimum conditions, experimental fatty acid methyl ester (FAME) content of 95.05 ± 0.26% was obtained, which was in good agreement with the predicted yield. The RSM model was developed using Box-Behnken design and the ANN predictive model was developed using a feed-forward backpropagation neural network algorithm with 14 neurons in the hidden layer. The mathematical models of RSM and developed ANN were compared for biodiesel yield. The higher value of correlation coefficient (R^2 = 0.99) and lower value of root mean square error (RMSE = 1.97) for ANN compared to RSM (R^2 = 0.95 and RMSE = 2.71) evidently proved that ANN model is far better in predicting FAME content compared to the RSM model.

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1. Introduction

Undoubtedly, depletion of easily accessible fossil fuels is currently one of the most challenging topics, which is gaining strict considerations during the past few decades. For this reason, biomass derived biofuels has emerged to be a priceless source primarily in the third-world economies [1]. Over the past several years, a number of research studies have been drastically addressed for the conversion of biomass into the high value-added products. In this regard, biodiesel is an invaluable product which is renewable and biodegradable. [2].

Generally, biodiesel is described as monoalkyl esters of long chain fatty acids that are produced by chemically reacting lipids [3]. Although there are several noteworthy advantages of biodiesel, the manufacturers are still facing various challenges in producing high-quality biodiesel with consistent characteristics, regardless of feedstock being used [4]. Over the years, a number of studies and researches have reported that base-catalyzed transesterification can produce high quality biodiesel in a short span of time. Moreover, base-catalyzed transesterification is the method by which most of biodiesel produced today is made. As reported by Wang et al. [5], base-catalyzed transesterification requires low temperature and pressure to produce high conversion yield with no intermittent compounds [5]. Previous research studies also validate that base-catalyzed transesterification can account for high conversion within a short span, usually ranging between 30 and 60 min [6–7].

Among different feedstocks available for biodiesel production, biodiesel production from highly polluting waste is of recent interest [8]. Waste cooking oil is one such waste that prohibits human improvement, and thus the social welfare [9]. Almost every nation in the world consumes million tons of edible cooking oil every year, out of which 20% is considered as waste, which could be possibly considered as a raw material for biodiesel production to cut down the petroleum imports [10]. Several research studies have reported that waste cooking oil is a promising feedstock for biodiesel production despite its disadvantages such as high free fatty acid and water contents. Moreover, a comprehensive review of the pre-treatment and the usage of waste cooking oil for the production of biodiesel using several techniques, different types of reactors, and various types and amounts of alcohol and catalysts have been reported in literature [11].

In the past decades, several mathematical tools have been developed for modeling and optimization. RSM and ANN are such tools suitable for modeling and simulation of real-world problems [12]. As reported by Jeong and Park [13], RSM can be used to optimize the process parameters of biodiesel production. This analysis by which the researchers were able to generate a multi level and multi factor RSM design and results disclosed that the generated model can predict the experimental range adequately. In another study carried out by Ferella et al. [14], RSM method established a good agreement between experimental and predicted yield of biodiesel which suggests that RSM is a useful tool to optimize the biodiesel yield.

ANN is a machine learning system to reproduce the neurological processing capability of the human brain [15]. Yuste and his coauthors [15] used ANN model to accurately simulate the production of biodiesel from Olive oil. The results depicted that ANN is a powerful tool to predict the experimental data. The similar observation was made by Ying et al. [16] in predicting biodiesel yield from Rapeseed soapstock.

Based on the above considerations, RSM and ANN have been widely used for modeling and optimization of biodiesel, but the predictive capabilities of both RSM and ANN have been rarely compared. Therefore, in the present work, RSM and ANN predictive models were developed and compared for the methanolysis reaction of waste cooking oil catalyzed by sodium hydroxide.

2. Materials and methods

2.1. Materials and chemicals

Waste cooking oil was collected from the college hostel mess and filtered using a muslin cloth to remove suspended solid impurities. After filtration, the oil is water degummed to remove trace impurities like protein, phosphatides, colorants, etc [17]. The procedure of degumming employed in this work is same as the method described by Araújo et al. [18]. After degumming, there was a notable reduction in acid value from 1.34 mg KOH/g to 1.21 mg KOH/g. All other necessary materials like anhydrous methanol, anhydrous sodium sulfate, and sodium hydroxide pellets were purchased from Merck Limited, India.

2.2. Biodiesel production and process conditions

The transesterification reaction was carried out in a batch type reactor with a base catalyst (NaOH) and methanol. The reactor was equipped with a stirrer and thermometer. The glass reactor vessel was maintained at fixed reaction temperature of 65 °C. The molar ratio of alcohol to oil was varied within the range of 3:1–9:1 with an interval of 3:1. The catalyst concentration was varied in the range of 0.75–1.25% (wt/wt) by an interval of 0.25%. The reaction time was varied within the range of 30 min to 90 min with an interval of 30 min and the stirrer speed was varied in the range of 300 rpm to 700 rpm with an interval of 200 rpm. The chosen range of process parameters is based on the suggestion made by Carlos et al. [19].

The transesterification reaction was carried out in an open system under barometric pressure. The required concentration of catalyst (NaOH) was initially dispersed in the oil under desired stirring speed and heated to reach the reaction temperature of 65 °C. Then, the required amount of pre-heated methanol was added to the mixture and the reaction was started. The reaction is carried out until the desired time and then the transesterified oil was transferred to a gravity separation funnel to separate crude or unpurified biodiesel and glycerol. The crude biodiesel was subjected to water wash method and finally, the refined biodiesel layer is collected for characterization and analysis of fuel properties.

2.3. Fuel properties and characterization

The critical fuel properties like density, viscosity, calorific value, cetane number, flash and fire point were determined experimentally by standard procedures. The acid value and saponification value of biodiesel was experimentally determined by titration procedure in accordance with EN 14104 and ASTM D 5558-95. The methanol content in biodiesel was determined in accordance with EN 14110 and water content by the Coulometric Karl Fischer method (EN 12937). Furthermore, free glycerin and total glycerin content in the test sample were estimated by method EN 14105. All the tests were done in duplicate and average values are presented.

The chemical composition of produced biodiesel was investigated by Fourier transform infrared transmission (FTIR) spectrum. The infrared spectrum of biodiesel was recorded on FT-IR-4100 type 'A' Spectrometer in the region of 4000–400 cm^{-1}. In this work, FTIR spectrum is used as a qualitative measurement to analyze the chemical structure of biodiesel.

2.4. Design of experiments

2.4.1. Response surface methodology

Since this work describes three-levels and four factors, Box-Behnken Design (BBD) is used for regression and graphical analysis of experimental data. In fact, BBD is a three-level experimental design for RSM in which each selection parameter is studied at three-levels with equally spaced interval [20]. The Minitab software (version 16.1.1) was used to