Shahid Bahonar University of Kerman

Agricultural Biotechnology Journal

Print ISSN: 2228-6705 Online ISSN: 2228-6500

Iranian Biotechnology Society

Optimizing the synthesis of biodiesel from jojoba oil using computational methods

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Abstract

Objectives

Different countries are interested in jojoba seed as a possible new energy source because it can grow well in harsh conditions like extreme weather, salty water, deserts, and high temperatures. Biodiesel is a fuel that can be used in motor engines, stoves, and home heating oil systems. It is recyclable, biodegradable, and safe. A cleaner-burning substitute for diesel fuel derived from petroleum, it is manufactured from animal fats, recycled cooking grease, or vegetable oils. Biodiesel (BD) is made in this study using jojoba oil under pressure. The inherent huge parallelism of neural networks (NNs) makes them a promising optimization tool. Commercial biodiesel production that is both efficient and environmentally friendly needs AI-powered process modelling and optimization.

Materials and methods

Predicting the ideal process parameters for biodiesel synthesis from jojoba oil was accomplished using artificial neural network-genetic algorithm (ANN-GA). With the help of the Integrated Artificial Neural Network - Genetic Algorithm (IANN-GA), this study aims to improve the transesterification process for changing Hyper Critical Methanol (HCM) into BD. The temperature range for IANN-GA optimization was 240–355°C, and the time range was set to 7–21 minutes.

Results

The primary composite design (PCD) for ANN modelling was used to create the initial studies. The best ANN structure with the right number of concealed neurons was found using a heuristic evaluation of the coefficient of determination (R) values. The R values obtained for training and testing demonstrate the high accuracy of the ANN framework.

Conclusions

The process variables for HCM transesterification have been optimized using GA with an ANN as the fitness coefficient. When taken as a whole, the findings demonstrated that ANN-GA is superior to the model that had been provided before, and that it is a trustworthy modeling and optimization approach for the manufacture of biodiesel from jojoba oil that is both practical and sustainable.

Keywords: Artificial Neural Network, Biodiesel synthesis, Genetic algorithm, Hyper critical methanol, Optimization

Paper Type: Research Paper.

Citation: Soy A, Tandan G (2024) Optimizing the synthesis of biodiesel from jojoba oil using computational methods. *Agricultural Biotechnology Journal* 16 (3), 229-242.

Agricultural Biotechnology Journal 16 (3), 229-242. DOI: 10.22103/jab.2024.24006.1614

Received: July 31, 2024. Received in revised form: September 27, 2024.

Accepted: September 28, 2024. Published online: September 30, 2024.

Publisher: Faculty of Agriculture and Technology Institute of Plant Production, Shahid Bahonar University of Kerman-Iranian Biotechnology Society.

Introduction

Scientists and researchers globally are investigating renewable, economically viable, and green energy sources due to the rising energy demands, limited fossil fuel reserves, and their harmful environmental effects (Emmanouilidou et al. 2024; Mishra & Kumar 2023). Various forms of renewable energy, including wave, wind PhotoVoltaic (PV), biological energy, and geothermal sources, have been effectively implemented (Martić et al. 2024; Ghotbaldini et al. 2019). Nevertheless, a limitation of certain forms of renewable energy, like wind and solar, is their intermittent availability (Nagarajan & Jensen 2010). Consequently, it is necessary to have energy storage equipment to store the energy (Veerasamy & Fredrik 2023). Researchers are investigating alternative materials that can store substantial energy in response to these factors (Abdolahimoghadam & Rahimi 2024; Ghufran & Huitink 2023). Of all the different types of renewable energy, biofuel is the easiest to handle because it is easy to transport and doesn't need to be stored. Another type of energy that can come from different places is BD, which can be made from vegetable oils (edible and non-edible), animal fats, and cooking oil waste (Mohd Johari et al. 2022). The production of biodiesel via the process of transesterification is a technique that is not only cost-effective and time-saving, but also results in fuel that has a higher cetane number and increased performance. BDs have a lot of potential because their physicochemical properties can be changed by carefully picking the feedstock and the steps used to make them, such as degumming, esterification, neutralization, transesterification, and cleansing. BD can also be mixed with other fuels, such as bioethanol and diesel, or the conditions under which they are made can be improved to make them even better. BDs have a lot of potential as diesel alternatives because they break down naturally, are safe, and release less harmful exhaust gases (Adenuga et al. 2021). BDs are mostly mono-alkyl esters from long chains of fatty acids. A process called esterification changes the free fatty acids in oils from plant or animal fats into esters. This is how the fuels are made. Transesterification is the next step. This is where the esterified oils react with short-chain ethanol with the help of a catalyst. To make BD (Silitonga et al. 2019; Aisien & Aisien 2023), alkalis, acidic substances, or enzymes are used as catalysts. In this work, sodium hydroxide has been used as a catalyst. Several mixtures of either acidic or alkaline catalysts are being created to produce BD, with varying levels of effectiveness. Typically, acid-catalyzed transesterification exhibits a relatively sluggish reaction rate, necessitating extended reaction durations. Additionally, there are challenges associated with retrieving the catalyst. Base-catalyzed transesterification is preferred in this case due to its faster speed and ability to decrease the oil's free fatty acids to less than one weight percent, resulting in higher BD yields (Topare et al. 2020; Goh et al. 2019). The BD yields are influenced by multiple factors, like the composition of fatty acids and physiochemical characteristics of the crude oils utilized as the raw material for BD production. Various types of operations can influence the BD synthesis process, and the order in which these processes are carried out can also impact the yields of BD (Ong et al. 2019; Mohammadabadi et al. 2024). The selected process parameters for BD synthesis (such as catalyst level, reaction period, alcohol-to-oil molar ratio, temperature, and mixing speed) have a known impact on BD yields (Yağız et al. 2022). A previous study (Zikri et al. 2020) showed that BD could be made using a two-step, lab-scale BD extraction method that included esterification and transesterification (Esonye et al. 2019). Over the course of the transesterification process that is used to produce biodiesel, sodium hydroxide serves as a catalyst to hasten the reaction that takes place among triglycerides found in oils and fats with methanol. Through the whole process of transesterification, the NaOH catalyst amount and the alcohol-to-oil molar ratio stayed at 1% by weight and 8:1, respectively (Jamil Muhammad Ammad 2024). As the results of the experiments showed, the synthesis rate of the C. manghas BD, which was 97.1%, was good enough. This rate changed depending on how much catalyst was used and how much alcohol was mixed with oil. In this study, we made an optimization model called IANN-GA to guess the process variables for changing the esters in jojoba oil (Das et al. 2021; Alireza et al. 2014; Selvaraju etal. 2019). Making a reliable forecasting model for the esterification and transesterification processes was important before starting the optimization process. Many studies have been done on how BD is made. However, little research has been done on using ANN computational modelling to look at the variables in the transesterification method. Moreover, data generation in agriculture and biotechnology has greatly increased in recent years due to the very rapid development of high-performance technologies (Mohammadabadi et al. 2024). These data are obtained from studying biological molecules, such as metabolites, proteins, RNA, and DNA, to understand the role of these molecules in determining the structure, function, and dynamics of living systems (Pour Hamidi et al. 2017). Functional genomics is a field of research that aims to characterize the function and interaction of all the major components (DNA, RNA, proteins, and metabolites, along with their modifications) that contribute to the set of observable characteristics of a cell or individual (i.e., phenotype). Furthermore, in a breeding program, genetic improvement can be maximized through accurate identification of superior organisms that are selected as parents of the next generation, thereby achieving breeding goals (Mohammadabadi et al. 2024). Artificial neural networks have been proposed to alleviate this limitation of traditional regression methods and can be used to handle nonlinear and complex data, even when the data is imprecise and noisy (Pour Hamidi et al. 2017). Agricultural data can be too large and complex to handle through visual analysis or statistical correlations. This has encouraged the use of machine intelligence or artificial intelligence (Ghotbaldini et al. 2019). To achieve the maximum yield of methyl ester, it is necessary to optimize the variables of the transesterification process. These parameters include the quantity of catalyst, reaction period and molar ratio of alcohol to oil, operating temperature, and mixing rate. By optimizing the process variables, the cost of BD production can be reduced, thereby increasing the competitiveness of BD fuels in the market. Thus, this study developed the IANN-GA model to forecast the optimal conditions for transesterification steps, and the model's accuracy has been evaluated. Biodiesel produced from jojoba oil and an examination of its physical and chemical characteristics will be discussed in the proposed model.

Materials and Methods

Synthesis of BD from Jojoba oil: Leven Rose, a company based in the USA, provided the jojoba oil utilized in this product.

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Methods for Collecting and Extracting Jojoba Oil: When harvesting jojoba seeds, be sure they are mature and clean before it try to extract their oil.

• Mechanical pressing followed by washing and drying is known as cold pressing, and it is a common approach for preserving natural qualities.

• Alternative method: solvent extraction, which may compromise purity and leave residues.

• Filtration: Primary and secondary filters for substance removal.

• Refinement: Bleaching and deodorization for highly scented and darkly colored products.

•To keep them from oxidizing, store them in transparent glass containers.

• Testing for Purity and Quality: Lab testing to ensure everything is up to par with industry requirements.

The oil is completely pure, natural, cold-pressed, and unprocessed. The process of transesterification was conducted using methanol ($CH3OH$). The $NaOH$ catalyst was acquired from Loba Chemie. Pretreatment was necessary to eliminate the water content from the crude Jojoba oil. To achieve this, the oil was subjected to heating at a temperature of 100 °C for one hour. Figure 1 presents a schematic diagram that provides a detailed representation of the sequential procedures involved in the synthesis of BD. This study's amount of Jojoba oil and temperature have remained constant. The $NaOH$ catalyst level has been adjusted, ranging from 1 to 1.5 weight percent. The response period and the ratio of moles were also altered, ranging from 20 to 85 minutes and from 1:1 to 8:1, respectively.

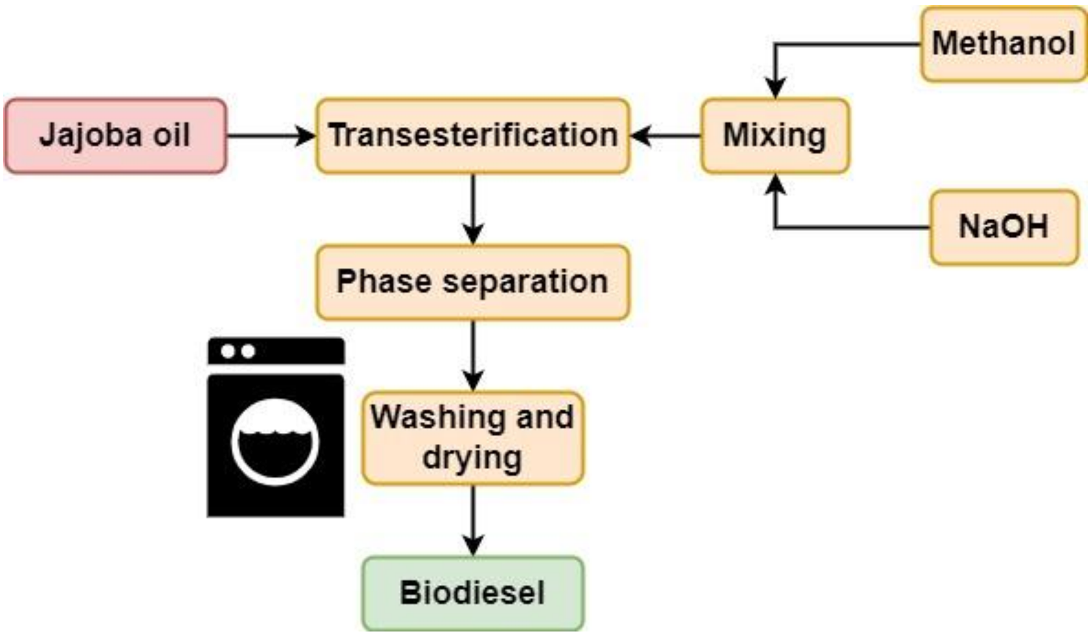

Figure 1. Synthesis of BD from Jojoba oil

For every experimental situation, the following steps have been followed: In the first step, the catalyst was thoroughly blended with methanol to generate sodium methoxide. Subsequently, the methoxide is combined with jojoba oil in a hermetically sealed container and subjected to specific duration and temperature conditions. The term used to describe this method is alkali transesterification. Following the specified duration, the mixture was transferred to a funnel to separate the glycerin. After glycerin is separated, the BD is rinsed with distilled water. Once the washing process is finished, the BD layer is heated to eliminate any remaining water and traces of methanol. The BD yield resulting from the steps mentioned above has been estimated in terms of volume percentage utilizing the volume equation provided in Equation (1):

$$Yield\ (\%) = \frac{Volume\ of\ BD}{Total\ feed\ volume\ (Jajoba\ oil + Methanol)} \quad (1)$$

HCM (Hyper Critical Methanol) transesterification process: The transesterification of Jojoba oil using HCM was conducted in an 85 mL spherical autoclave continuous reactor vessel made of stainless steel. The reactor used had been fitted with a stirrer and a temperature sensor. For every experiment, the reactor was filled with different mixtures of methanol and Jojoba oil, with compositions ranging from 12:1 to 24:1. The reactor vessel was heated using a thermostat aluminium plate jacket and kept at a predetermined temperature for a set duration. The chosen temperature range was 240–355°C, and the selected period was 7–21 minutes. The reaction mix was agitated incessantly utilizing a magnetic stirring bar. The process was not subjected to any external pressure; instead, the temperature solely created the pressure. Following the designated period, the reactor was immersed in an ice-water bath to suppress additional reactions. The BD transformation was determined by evaporating the remaining methanol in the product employing a rotavapor and then calculating it.

Transesterification process for converting HCM into BD using IANN-GA optimization: Combining the advantages of Genetic Algorithms (GAs) with Artificial Neural Networks (ANNs) produces a robust optimization framework. The advantages and operation of this integration are summarized below:

Artificial Neural Networks: Artificial neural networks (ANNs) are computer models that perform operations similar to the human brain, such as pattern identification, classification, and regression. Using back-propagation to alter weights, they learn from data.

GA Algorithms: Genetic algorithms (GAs) are optimization methods that draw on genetics and natural selection. They take part in a population of solutions and use processes like mutation, selection, and crossover to improve them over time.

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Modelling and optimizing the HCM process: An ANN model was developed using the experimental runs recommended by the PCD. Before modeling, the ANN information was normalized to expedite the training process and avoid any imbalances in data flow caused by extremely large or small weights. It also prevents the network from reaching local optima. The information was normalized using the following Equation:

$$Normalized = \left[\frac{2(Dreal - Dlow)}{(Dhigh - Dlow)}\right] - 1] \quad (2)$$

where $Dreal$, $Dlow$, and $Dhigh$ represent the values of the real, lowest, and highest information, respectively. Normalization transforms data into values between 1 and -1, representing the lowest and highest levels. In this case, the tangential sigmoid function ($tansig$) was chosen for modeling, as it also has the same range. Therefore, a three-level Lavenberg–Marquardt (LM) back-propagation algorithm was utilized, with a $tansig$ activation function on the concealed layer and an exponential function ($pureexp$) on the output layer. Because this algorithm is having efficient learning, better activation function, robustness and efficiency. This choice was made because it resulted in a lower MSE and variance, along with the largest R values. The number of neurons in the concealed layer is crucial in constructing an ANN model. Excessive or insufficient neurons can lead to underfitting or overfitting of information, which may result in the inability of the network to accurately determine the relationships between patterns and interpret the signals in the database. The neurons in the concealed layer have been optimized using heuristic analysis to determine a highly efficient network architecture that would yield the most accurate predicted results. The number of neurons chosen for optimization ranged from 3 to 25. We have built the proposed model in MATLAB 2020A with the I5 installation. MATLAB is a platform and programming language used by scientists and engineers for system and product creation and analysis. Instead of dealing with raw numerical values, this high-level language makes use of matrices and arrays. To create an ANN model, the data from the experiment was divided into two groups: training and testing information, using an arbitrary method. The training of the ANN involved randomly selecting 70% of the data. The remaining 30% of the information was then used to test the ANN using the weighted characteristics obtained during the training phase. Several hypothesis tests were performed to assess the model's accuracy level, including the t-test to compare means, the F-test to compare variances, and Levene's test to assess variance equality.

GA optimization: Once an appropriate ANN model was developed, GA was utilized to optimize the transesterification operations in the proposed IANN-GA optimization. The suggested model has an R-value of 98%, as seen in Figure 3. Good fits and strong correlations between experimental and projected values are supported by the models' low error indices and high R values. The GA starts with an initial population deliberately selected to cover the entire range of input parameters. This is done to avoid the risk of the algorithm converging to a local minimum. GA iteratively enhances individuals by evaluating their fitness to generate superior offspring in subsequent generations. This leads to the most exceptional individuals evolving in the following generation and converging towards the most recent solution. The individuals were classified based on their level of physical fitness and then underwent three operations: selection, crossover, and mutation. After the completion of the process, the individual with the highest fitness level will be replaced by the individual with the lowest fitness level in the original population, creating a new population. This process generated a more effective solution in each subsequent generation. After multiple generations, the algorithm reached a point of convergence, and the most successful individual had evolved, representing the optimal solution.

Results and discussion

All experimental trials devised by PCD were carried out in controlled laboratory settings, and the outcomes of the BD conversion utilizing IANN-GA optimization are depicted in Fig. 2. The ANN modeling was performed using the experimental data presented in Figure 2.

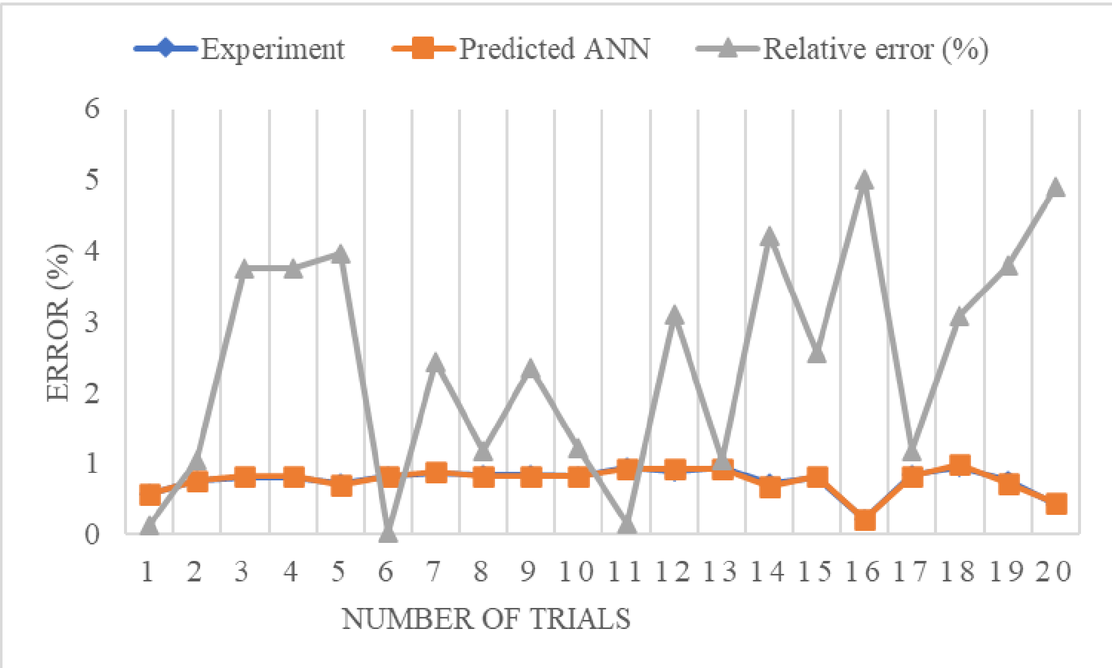

Figure 2. Experimental and predicted modeling for varying number of trials using IANN-GA for BD synthesis

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The number of neurons in the concealed layer plays a crucial role in constructing a suitable IANN-GA model. The number of neurons in the concealed layer was optimized by performing heuristic evaluation on the R values displayed in Figure 3. The range of neurons considered was between two and twenty. The ideal number of concealed neurons identified was eight, with a maximum R-value of 0.999 and 0.998 for the training and testing sets, respectively.

The equation for calculating R value is given in below Equation

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(Y_{ip} - Y_{ie}\right)^2}{\sum_{i=1}^{n}\left(Y_{ip} - Y_{e}\right)^2}$$

Here, Values from experiments, predictions, the average of those values, and the total number of runs are denoted by Yie, Yip, Ye, and n, respectively.

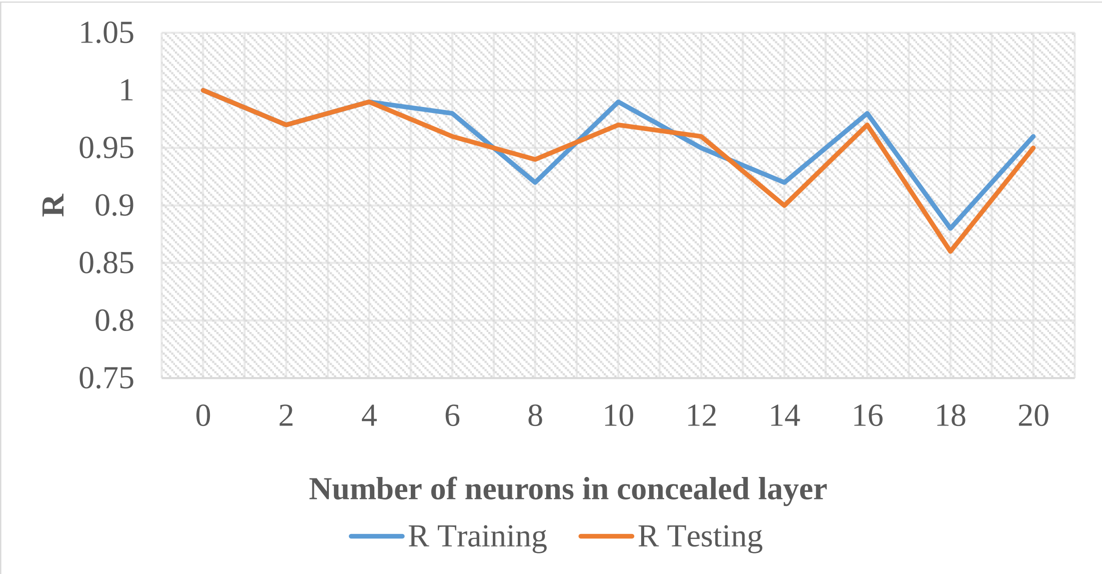

Figure 3. Heuristic evaluation on the R values using IANN-GA for BD synthesis

Process optimization revealed that a biodiesel yield of 87.84 wt% was achieved with ANN-GA optimal conditions tested at 89.67 wt%. The maximum experimental yield of 88.5% is lower than some values reported in the literature (Milano et al. 2018), but it is higher than 70wt% reported by other authors on optimizing jatropha curcas using heterogeneous catalysts (Jamil Muhammad Ammad 2024). It is also within the same range as 89.85wt% (Dominic Okechukwu Onukwuli et al. 2021) and 87.10wt% (Ajiwe VIE et al. 1997) observed for optimizing neem oil and immobilized lipase-catalyzed transesterification of jatropha curcas oil, respectively. The fact that various feedstocks include varying amounts of monoglycerides, diglycerides, and triglycerides may account for these differences.

Conclusion: The present study employs pressurized jojoba oil for the production of BD. This study aims to enhance the transesterification process of converting HCM into BD by employing an Integrated Artificial Neural Network - Genetic Algorithm (IANN-GA). The selected process parameters for IANN-GA optimization consisted of a temperature range from 240 to 355°C and a time range from 7 to 21 minutes. The initial investigations were conducted using the PCD for ANN modeling. The optimal ANN architecture, with an appropriate number of hidden neurons, has been identified using heuristic assessment of the coefficient of determination (R) estimates. The ideal number of concealed neurons identified was eight, with a maximum R-value of 0.999 and 0.998 for the training and testing sets, respectively. The process variables for HCM transesterification have been optimized using GA with an ANN as the fitness coefficient. Less energy and power consumption, a high production rate, and a decrease in the necessity for raw materials would be the end result. Using renewable and environmentally friendly underused African star apple seed oil in this way allows for the long-term manufacture of high-quality methyl ester. Several ANN models will be used for optimization in the future.

Conflict of Interest: There is no conflict of interest.

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Agricultural Biotechnology Journal; Print ISSN: 2228-6705, Electronic ISSN: 2228-6500

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مجله بیوتکنولوژی کشاورزی
انجمن بیوتکنولوژی ایران
شاپا چاپی: ۶۷۰۵-۲۲۲۸ شاپا الکترونیکی: ۶۵۰۰-۲۲۲۸

بهینه‌سازی سنتز بیودیزل از روغن جوجوبا با استفاده از روش‌های محاسباتی

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تاریخ دریافت: ۱۴۰۳/۰۵/۱۰ تاریخ دریافت فایل اصلاح شده نهایی: ۱۴۰۳/۰۷/۰۶ تاریخ پذیرش: ۱۴۰۳/۰۷/۰۷

چکیده

هدف: کشورهای مختلف به دانه جوجوبا به عنوان یک منبع جدید انرژی علاقه‌مند هستند زیرا می‌تواند در شرایط سخت مانند آب و هوای شدید، آب شور، بیابان‌ها و دمای بالا به خوبی رشد کند. بیودیزل سوختی است که می‌تواند در موتورهای خودروها، اجاق گاز و سیستم‌های گرمایش روغنی خانگی استفاده شود و قابل بازیافت، زیست تخریب‌پذیر و ایمن است. یک جایگزین سوخت پاک کننده برای سوخت دیزل که از نفت بدست می‌آید است و از چربی‌های حیوانی، گریس پخت و پز بازیافت شده یا روغن‌های گیاهی تولید می‌شود. بیودیزل (BD) در این مطالعه با استفاده از روغن جوجوبا تحت فشار ساخته شده است. پاراللیسم عظیم ذاتی شبکه‌های عصبی (NN) آن‌ها را به یک ابزار بهینه‌سازی امیدوارکننده تبدیل می‌کند. تولید بیودیزل تجاری که هم کارآمد و هم سازگار با محیط زیست باشد، نیازمند مدل‌سازی و بهینه‌سازی فرآیند مبتنی بر هوش مصنوعی است.

مواد و روش‌ها: پیش‌بینی پارامترهای فرآیند ایده‌آل برای سنتز بیودیزل از روغن جوجوبا با استفاده از الگوریتم ژنتیک شبکه عصبی مصنوعی (ANN-GA) انجام شد. با کمک شبکه عصبی مصنوعی یکپارچه - الگوریتم ژنتیک (IANN-GA)، این مطالعه با هدف بهبود فرآیند ترانس استریفیکاسیون برای تبدیل متانول فوق بحرانی (HCM) به BD انجام شد. محدوده دما برای بهینه سازی IANN-GA برابر ۳۵۵-۲۴۰ درجه سانتیگراد بود و محدوده زمانی روی ۷-۲۱ دقیقه تنظیم شد.

نتایج: طراحی ترکیبی اولیه (PCD) برای مدل‌سازی ANN برای ایجاد مطالعات اولیه استفاده شد. بهترین ساختار ANN با تعداد مناسب نورون‌های پنهان با استفاده از ارزیابی اکتشافی مقادیر ضریب تعیین (R) پیدا شد. مقادیر R به دست آمده برای آموزش و آزمایش دقت بالای چارچوب ANN را نشان می‌دهد.

نتیجه‌گیری: متغیرهای فرآیند برای ترانس استریفیکاسیون HCM با استفاده از GA با ANN به عنوان ضریب تناسب بهینه شدند. به طور کلی، یافته‌ها نشان داد که ANN-GA نسبت به مدلی که قبلا ارائه شده بود برتر است و این یک رویکرد مدل‌سازی و بهینه‌سازی قابل اعتماد برای ساخت بیودیزل از روغن جوجوبا است که هم عملی و هم پایدار است.

واژه‌های کلیدی: الگوریتم ژنتیک، بهینه سازی، سنتز بیودیزل، شبکه عصبی مصنوعی، متانول فوق بحرانی

نوع مقاله: پژوهشی.

استناد: سویا آکانشا، گاجندرا تاندان (۱۴۰۳) بهینه‌سازی سنتز بیودیزل از روغن جوجوبا با استفاده از روش‌های محاسباتی. *مجله بیوتکنولوژی کشاورزی*، ۱۶(۳)، ۲۲۹-۲۴۲.

Publisher: Faculty of Agriculture and Technology Institute of Plant Production, Shahid Bahonar University of Kerman-Iranian Biotechnology Society.