

An artificial intelligence approach to model and optimize biodiesel production from waste cooking oil using life cycle assessment and market dynamics analysis

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ABSTRACT

Biodiesel has emerged as a viable alternative to fuel, offering a more sustainable and environmentally friendly energy option. The current study explores the modeling and optimization of biodiesel production from waste cooking oil using artificial intelligence and genetic algorithms. The study focuses on enhancing five process parameters: methanol-to-oil molar ratio, catalyst concentration, reaction temperature, reaction time, and stirring speed. The optimization of these parameters is complemented by a life cycle assessment to reduce environmental impact. The approach considers biodiesel yield, high heating value, and energy consumption as output variables, thereby advancing sustainable biodiesel production. The findings indicated that, under optimal conditions (methanol-to-oil ratio of 1:6.9, stirring rate of 500 rpm, reaction duration of 20 s, reaction temperature of 30 °C and catalyst concentration of 1), the transesterification process achieved the maximum biodiesel yield of 97.76 %. The optimization reached a low environmental impact in the production of biodiesel in an efficient way. Additionally, SWOT analysis helps to develop strategic methods that can enhance efficiency and increase competitiveness. The research suggests that, by optimizing the chemical process in biodiesel production, it is possible to achieve a high yield and high heating value of the biofuel, along with feasible environmental mitigation strategies.

1. Introduction

Energy is a fundamental requirement for the economic progress of any country. Fossil fuels like crude oil and coal serve as the main energy source. However, the extensive use of crude oil has become of significant socioeconomic concern, especially for nations that have limited crude oil reserves. This situation has caused a rise in crude oil prices, causing global economic instability [1]. This prompts a pursuit of alternative, renewable, and cleaner energy sources directed at reducing reliance on fossil fuels and curbing greenhouse gas emissions. Among these alternatives, biodiesel, a type of biofuel, has emerged as particularly noteworthy [2]. One goal of the European Green Deal (EGD) is to cut greenhouse gas emissions. More than 75 percent of greenhouse gas emissions in the EU are caused by the use and production of energy [3]. Therefore, decarbonizing the EU energy system is essential to meet the

EU's long-term plan to achieve carbon neutrality by 2050 and to reach our 2030 climate objectives. Furthermore, the EU strove to have even greater ambition and action in this crucial decade during the 28th UN Climate Change Conference (COP28) climate discussions. It sought to phasing out fossil fuels and boosting the capacity of renewable energy sources and energy efficiency [4].

Biodiesel typically undergoes a transesterification process in which a triglyceride, such as fat or oil, reacts with an alcohol in the presence of a catalyst. Currently, the main method to produce biodiesel involves homogeneous catalysis, in which a basic catalyst, such as potassium hydroxide (KOH) or sodium hydroxide (NaOH), is dissolved in methanol [5]. The resulting biodiesel exhibits nearly identical properties to those of conventional diesel fuel, including energy content, viscosity, and phase characteristics. Consequently, it can be seamlessly integrated into diesel engines with minimal adjustments or, in some cases, no

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modifications at all [6]. Researchers have conducted in-depth studies of biodiesel and other potential alternatives to reduce reliance on crude oil. Alternative fuels refer to substances resembling fossil fuels in their properties and efficiency of use [7]. Biodiesel, produced from vegetable oils or animal fats, is a methyl ester that is employed as a fuel for diesel engines [8]. The most important raw materials include waste oils such as waste cooking oil (WCO) [9]. WCO can be repurposed by recycling it through a transesterification process to create biodiesel. Employing WCO as a biodiesel feedstock offers a solution to problems like water contamination and blockages in drainage systems, which reduces the need for additional cleaning [10]. While numerous studies have highlighted the environmental advantages of biodiesel compared to fossil fuels [11], it is important to recognize that biodiesel can also pose certain adverse impacts on the environment [12]. This approach proves to be highly efficient in addressing disposal concerns while partially meeting the global energy demand [13]. However, the interest in evaluating the costs and environmental impact of biodiesel production arises from concerns that are related to energy consumption, pollutant emissions, and the depletion of natural resources due to these production processes [14]. In line with the foregoing, effective exploration of renewable energy sources has been undertaken to mitigate the adverse impacts of CO₂ emissions and other greenhouse gases that result from the use of fossil fuels [15].

Machine learning, a component of artificial intelligence (AI), operates on the principle of autonomous learning, enabling computers to learn without explicit programming. With sufficient training data, these algorithms discern patterns, assimilate knowledge, and draw conclusions [16]. The decision to employ a machine learning algorithm is rooted in its capability to uncover intricate connections among diverse input parameters that can often exhibit nonlinear or polynomial associations [17]. The model's adeptness in comprehending these intricate relationships dictates its effectiveness in predicting outcomes. Similar to AI and machine learning methodologies, the adoption of genetic algorithms (GA) has been embraced increasingly beyond traditional computer science applications [18]. Recently, the application of AI in biodiesel production has revolutionized the optimization of the transesterification process [19]. Enhancing biodiesel yield in the transesterification process involve optimizing key processing factors. These include methanol/oil ratio, catalyst concentration, stirred rate, and reaction time [20]. Additionally, other factors impact the sustainability of biodiesel produced from waste cooking oil, including the collection process of the used oil [21]. However, because conducting experimental optimization often requires expensive and time-consuming laboratory tests, there was a need to devise a method would require fewer experimental runs while optimizing biodiesel production parameters [19]. The integration of IA with genetic algorithms (GA) emerged as a contemporary and highly effective approach for this purpose [22]. These cost-effective methods, can enhance efficiency and reduce biodiesel production costs from waste oil. They offer a more sustainable alternative to fossil fuels. This AI-driven approach not only streamlines the production process, but also contributes significantly to sustainable energy practices, thus paving the way for advancements in environmentally friendly fuel production methodologies [23].

Optimization techniques, such as linear regression, response surface methodology (RSM), and ANN, have been employed to enhance the transesterification process by increasing the yield and HHV. Previous research papers on biodiesel production optimization have explored various approaches to maximize biodiesel production. These methods have been leveraged due to their ability to model and optimize complex systems, thus aiding the efforts to maximize biodiesel production. Kumar et al. [24] emphasized that Response Surface Methodology (RSM) stands out as the widely preferred statistical technique to optimize the variables involved in the transesterification process in biodiesel production. Studies conducted by Vinoth et al. [25] utilized ANN methodology to optimize the biodiesel production parameters. While the work of Vinoth Arul Raj et al. [26], Soji-Adekunle et al. [27], and

other researchers, delved into optimizing the parameters of the biodiesel production process employing both ANN and RSM techniques. Existing references have not used regression models based on machine learning (ML) and Genetic Algorithms (GA) to optimize output variables, such as yield and HHV in biodiesel production from WCO. This reveals a significant gap in research. It indicates an untapped avenue for enhancing biodiesel production efficiency.

The existing literature emphasizes that the primary focus in biodiesel production concerns performance. This encompasses the experimental design's response in both parametric and optimization studies [28]. However, this emphasis solely on performance may overlook essential aspects due to the energy intensive nature of biodiesel production, as well as its generation of waste. Hence, aside from production yield, it is necessary to account for and prioritize energy consumption and waste generation during any optimization of the transesterification process [29]. Integrating these factors into the optimization strategy is consistent with the principles of sustainability and environmentally friendly practices.

Life Cycle Assessment (LCA) has been used extensively in comparing the environmental sustainability of bio-based and fossil-based products [30]. LCA examines the environmental repercussions of a product or process from inception to utilization, facilitating comparisons of environmental hotspot sources and triggers, thereby aiding decision makers and policy makers in devising solutions [31]. Several researchers have conducted extensive Life Cycle Assessment (LCA) studies on various biodiesel production processes. These include comprehensive investigations of different feedstocks, such as waste cooking oil [32]. These LCA studies yield diverse outcomes due to variations in system boundaries, functional units, and study objectives. Typically, these assessments focus solely on energy balance and greenhouse gas emissions. However, this work takes a more comprehensive approach by a thorough LCA in lab scale for this biodiesel production. Because of this has been made a midpoint and endpoint indicator assessment. Understanding the implications between these categories is necessary for a holistic evaluation of the environmental impact of biodiesel production.

Also, the complexity of biodiesel production systems leads to significant outcome variations due to differences in input data and geographical contexts [33]. Data availability and precision present significant challenges, as the accuracy and outcomes of the Life Cycle Assessment (LCA) model depend on the quality of input data. These challenges contribute to knowledge gaps in waste cooking oil-based biodiesel production, particularly regarding optimal operating parameters and their environmental implications. Additionally, there is limited understanding of the interactions among various input factors, such as feedstock characteristics and process parameters. The absence of standardized methodologies further complicates comparative analysis and definitive conclusions.

Addressing these knowledge gaps is necessary in order to devise effective strategies and decision-making processes that will improve biodiesel yield and reduce environmental impact. Therefore, in this study, the concurrent influence effects of catalyst concentration, methanol-to-oil molar ratio, reaction time, stirred rate, and temperature were explored. This involved the use of models of WEKA (Waikato Environment for Knowledge Analysis) that employed algorithms and approaches. From this comprehensive suite, models that exhibited the fewest errors were chosen for each output variables. This ensured the most accurate predictive performance. The interaction effects between the reaction variables were examined and those variables that affect the transesterification process most significantly were optimized using GA. Then, a life cycle assessment was conducted based on the optimized values. Finally, a SWOT analysis was conducted to gain deeper understanding of the use of waste cooking oil for biodiesel production, in the hope of reducing its environmental and human impact (Fig. 1). These efforts to enhance biodiesel yield and HHV while minimizing energy consumption, specifically by reducing the reaction temperature, the

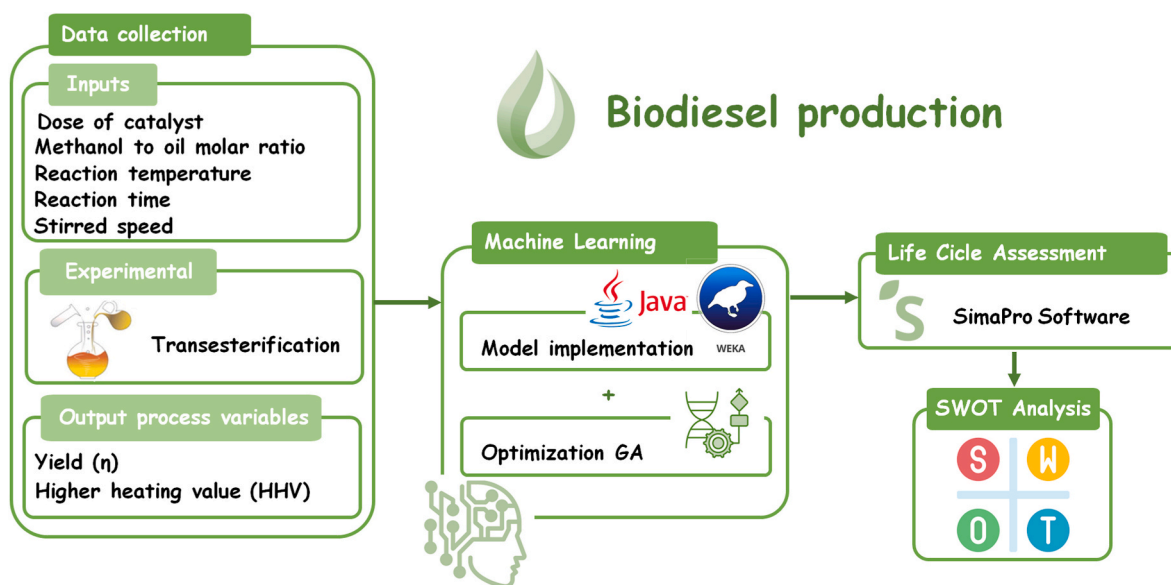


Fig. 1. Methodological workflow.

reaction time, and the speed of the production process. Additionally, we have endeavored to identify and address the current gaps and forthcoming challenges within this domain, with the aim of enhancing the economic viability of the biodiesel production process. The uniqueness of this study lies in its strategy for creating an environmentally efficient biodiesel production method and assessing its environmental impact by Life Cycle Assessment (LCA) criteria. The production of biodiesel from waste cooking oil contributes to decreasing the disposal of such oil, which is considered to be hazardous waste according to European Union standards.

2. Materials and methods

2.1. Materials

The WCO that in the biodiesel production process used was collected from a restaurant at La Rioja University, in Logroño (La Rioja, Spain). These samples were collected in plastic containers, homogenized, and stored under ambient temperature and atmospheric pressure. It was essential to eliminate solid particles and water present in the oil. Accordingly, the oil was heated to 120 °C for 12 min to reduce the water content [34]. Then, the oil was filtered using a cellulose filter to remove residues before use.

The methanol (CH₃OH, 99.8 % extra-pure, CAS: 67-56-1) and sodium hydroxide (NaOH, 98 % extra-pure, CAS: 1310-73-2) that were needed for the transesterification process were sourced from Merck Co., Ltd. (Darmstadt, Germany).

2.2. Experiments design

Design of Experiments (DoE) is a statistical approach employed to investigate the relationships between several input parameters and one or more output (response) variables. This methodology helps in identifying which variables most significantly affecting the output and in determining their optimal values. Moreover, DoE aims to minimize the number of experiments or data points required to obtain reliable results. A Box-Behnken Design (BBD) was used, with the intention of validating initial hypotheses with minimal data. A BBD is a form of fractional factorial design that allows the effect of multiple independent variables on a response or dependent variable to be evaluated, with a relatively low number of trials compared to a full factorial design. This makes it ideal for optimizing processes and reducing costs and time in

experimentation [35].

Utilizing BBD as the foundation, Table 1 details parameter values and levels necessary for executing the DoE. These variable ranges, drawn from referenced sources [36–39] were chosen carefully to encompass existing literature and thus foster a comprehensive exploration of the variables under investigation.

Stat-Ease 360 Design Expert Version 7.1.6 (Stat-Ease, USA) was used to generate a design matrix for the biodiesel production process, emphasizing five input parameters. The parameters were catalyst dose (A), methanol-to-oil molar ratio (B), reaction temperature (C), reaction time (D), and stirring speed (E). They are shown in Table 2. These parameters varied systematically in three levels (−1 for low, 0 for the midpoint, and +1 for high) within the Box-Behnken Design (BBD) framework. This resulted in a matrix of 33 distinct experiments. The creation of this matrix followed the definition of specific parameters and their corresponding values for biodiesel production.

2.3. Experimental procedure

Biodiesel was manufactured in a laboratory setting by the transesterification process, employing methanol, waste cooking oil, and NaOH as catalyst. The transesterification process was carried out in a 250 mL flat-bottom flask, which held 50 mL of waste oil. This flask was set on a magnetic stirrer coupled with a heated plate. During the reaction, a Metrix PX-120 digital multimeter (Metrix, Chauvin Arnaud, France) was used to monitor the power consumption (W) of the magnetic hot stirrer. Following completion of transesterification, the stirring and heating were ended. The newly produced biodiesel was washed with deionized water to eliminate residual alcohol, catalyst, and reaction byproducts. A quantity of cleaning that water equal to 60 wt% of the biodiesel was used [40]. Subsequent tests were conducted according to

Table 1
Input process parameters and their respective levels for the process.

Input/Units	Code values	Levels		
		−1	0	1
Catalyst dose [wt.%]	A	1.0	1.5	2.0
Methanol to oil molar ratio [mg/L]	B	6.0	7.5	9.0
Reaction temperature [°C]	C	20.0	30.0	40.0
Reaction time [s]	D	20.0	30.0	40.0
Stirred speed [rpm]	E	500	750	1000

Table 2

Reaction conditions and η and HHV results of transesterification based on the Box–Behnken design.

Run n°	Input process parameters (code values)					Outputs process variables	
	A	B	C	D	E	η	HHV
	(wt.%)	(mg/L)	(°C)	(s)	(rpm)	(%)	(MJ/kg)
1	1.0	6	30	30	500	0.93	42.70
2	1.0	6	30	30	1000	0.93	41.83
3	2.0	6	30	30	500	0.40	42.06
4	1.5	6	30	30	1000	0.95	41.78
5	1.5	6	20	20	750	0.29	41.94
6	1.5	6	40	20	750	0.29	42.19
7	1.5	6	30	30	750	0.79	42.32
8	1.5	6	20	40	750	0.31	41.61
9	1.5	6	40	40	750	0.57	42.87
10	1.0	9	30	30	500	0.88	43.99
11	1.0	9	30	30	1000	0.55	42.26
12	2.0	9	30	30	500	0.50	43.72
13	2.0	9	30	30	1000	0.23	42.40
14	1.5	9	20	20	750	0.59	42.30
15	1.5	9	40	20	750	0.91	43.13
16	1.5	9	30	30	750	0.84	42.83
17	1.5	9	20	40	750	0.85	42.29
18	1.5	9	40	40	750	0.82	42.30
19	1.0	7.5	30	20	750	0.91	43.41
20	1.0	7.5	20	30	750	0.94	43.11
21	1.0	7.5	40	30	750	0.89	43.30
22	1.0	7.5	30	40	750	0.92	43.63
23	2.0	7.5	30	20	750	0.75	40.48
24	2.0	7.5	20	30	750	0.34	42.06
25	2.0	7.5	40	30	750	0.23	41.93
26	2.0	7.5	30	40	750	0.78	41.72
27	1.5	7.5	30	20	500	0.88	42.65
28	1.5	7.5	30	20	1000	0.97	42.33
29	1.5	7.5	20	30	500	0.87	43.09
30	1.5	7.5	40	30	500	0.86	42.21
31	1.5	7.5	30	20	1000	0.83	44.14
32	1.5	7.5	30	40	1000	0.92	42.30
33	1.5	7.5	40	30	500	0.83	42.65

Table 2 to determine the yield (η) and higher heating value (HHV) of the washed biodiesel.

The biodiesel yield, which indicates the percentage mass ratio of the biodiesel generated to the total mass of the waste cooking oil used is determined by Equation (1).

$$\text{Yield (\%)} = \frac{W_{\text{biodiesel}}}{W_{\text{WCO}}} \cdot 100 \quad (1)$$

where $W_{\text{biodiesel}}$ is the weight of biodiesel after transesterification process and W_{WCO} is the weight of waste cooking oil used for the transesterification process. All the experiments trials were conducted in triplicate to ensure consistency and reduce variations in the findings of the analysis. The relative deviation was maintained within the order of $\pm 1.5\%$, and the average results were presented.

The high heating value of the biodiesel sample was determined by a bomb calorimeter (PARR).

1351 Bomb Calorimeter; Parr Instrument, USA) following the ASTM D240 standard.

2.4. Machine learning regression models description

Following the establishment of the Design of Experiments (DoE) and subsequent laboratory tests, prediction models were formulated by use of input parameters and the results of tests. The development of regression models in this study was facilitated by the use of machine learning.

The implementation of, WEKA (Waikato Environment for Knowledge Analysis), version 3.9.5, open-source machine learning software, a product of the University of Waikato Hamilton, New Zealand, stands as a

comprehensive suite. It comprises diverse machine learning methodologies that are tailored to resolve the complexities inherent in data mining endeavors. WEKA is equipped with tools for data pre-processing, regression, classification, association rules, clustering, and visualization. It includes a variety of open-source machine learning algorithms that are designed to address practical data mining challenges. Its meticulous process ensures the accuracy and reliability of the models. Initially, the database underwent a normalization process. This was pivotal to align the scale of various data parameters and thereby mitigate any potential bias arising from disparate data magnitudes. Following the normalization, the Randomize filter was applied. This step was crucial in randomizing the instances within the database, which serves a dual purpose. Primarily, it helps to prevent the training algorithms from conforming to local trends, which might skew the model's performance. Secondly, it ensures the development of robust regression models that are capable of capturing and generalizing global-level behaviors. Following randomization, the database was bifurcated using the StratifiedRemoveFolds filter or fold for cross validation. This division allocated 75 % of the data for training and validation purposes, while reserving the remaining 25 % available for testing. Such a stratified approach guarantees a representative distribution of data across training and testing sets. This is essential to maintain the integrity of the model evaluation process.

WEKA played a pivotal role in the model generation process. Employing advanced prediction algorithms is imperative to ensure precise handling of complex interdependencies and effective management of correlated variables. In this study, algorithms from the following groups were used for modeling the yield and HHV: (i) neural network models, (ii) statistical models, (iii) linear models, (iv) decision trees, (v) lazy methods and (vi) rules. Further, in the quest to identify the most optimal model, AutoWEKA (run for 360 min) was employed. AutoWEKA is instrumental in automating the model selection process. This approach is particularly effective in sifting through various models to identify the one that exhibits the best performance on the given dataset. In the final phase, the model adjudged as the best by AutoWEKA underwent a manual testing process. Here, the focus was on validating the model's efficacy by computing the testing error on the 25 % of data earmarked for testing. This step is vital to confirm the model's accuracy and its ability to generalize beyond the training dataset, and thereby ensure its applicability in real-world scenarios. By means of this comprehensive process, we have sought to develop machine learning regression models that are not only accurate in their predictions, but also robust and reliable in their application.

To identify the most effective machine learning algorithm for optimizing biodiesel production parameters, the proposed models were subjected to a training and testing regimen, culminating in a comparative assessment of their performance. In this research, the algorithms were applied directly to the collected dataset. Validation of the models was conducted during the testing phase to confirm their broad applicability. The final step involved optimizing the chosen model to ensure the best possible outcomes.

2.5. Performance metrics

The machine learning models' performance was assessed using three performance indicators: Correlation Coefficient (Corr), Root Mean Square Error (RMSE), and Mean Absolute Error (MAE). These indicators were computed using of Equations (2)–(4).

$$\text{Corr} = \frac{\sum_{a=1}^N (Y_{a \text{ Experiment}} - \bar{Y}_{\text{Experiment}})^2 (Y_{a \text{ Experiment}} - \bar{Y}_{\text{Model}})^2}{\sqrt{\sum_{a=1}^N (Y_{a \text{ Experiment}} - \bar{Y}_{\text{Model}})^2 \sum_{a=1}^N (Y_{a \text{ Experiment}} - \bar{Y}_{\text{Model}})^2}} \quad (2)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{a=1}^N (Y_{a \text{ Experiment}} - Y_{a \text{ Model}})^2} \quad (3)$$

$$MAE = \frac{1}{N} \sum_{a=1}^N |Y_{a \text{ Experiment}} - Y_{a \text{ Model}}| \quad (4)$$

where $Y_{\text{Experiment}}$ are the outputs obtained experimentally, whereas Y_{Model} are outputs of the models, \bar{Y} is the mean of observed values in Y variables and N is the total number of experiments.

2.6. Optimization based on genetic algorithms (GA)

Genetic algorithms (GAs) represent a powerful heuristic search technique. They were inspired by the natural selection mechanism of evolution [41] and are widely utilized in the field of artificial intelligence. Their primary role is to seek optimization solutions in scenarios where conventional methods grapple with complexity, such as situations involving a substantial number of variables to optimize or highly nonlinear problems saturated with constraints [42]. Using genetic algorithms enables the discovery of solutions that may not be obvious or intuitive. This approach can lead to fresh perspectives and enhance the efficiency and effectiveness of various processes, such as biodiesel production [43]. Predictive models were created as depicted in Section 2.3, being for Weka the basis of its training and also of the evaluation of each instance of the GA's population. In this work (Fig. 2), the initial step was to create an initial population by indicating the number of input parameters, their names, and ranges. The initial population size was determined to be sufficient to cover the entire search space without incurring excessive computational costs. Typically, this population is generated by random combinations, although it can also be introduced using heuristic techniques [44]. In this case, the study involved 100 individuals. Additionally, the output variables yield and HHV were defined along with their ranges. The final part of this stage involved defining the preset objectives for the algorithm to achieve. These objectives were to increase the yield (η) and the heating value (HHV) of the biodiesel obtained, while minimizing catalyst dose (A), methanol-to-oil molar ratio (B), reaction temperature (C), reaction time (D), and stirring speed (E) considered for its production. Furthermore, an objective function, J_i , was established to assess the difference between the preset

objectives and the output variables, yield and HHV, derived from the predictive models, alongside their respective input parameters. This objective function (see Equation (5)) was defined as the sum of all absolute errors between these predicted outputs and the target values (A, B, C, and E) to be minimized, as listed in Table 4.

$$J_i = |\eta_{\max} - \eta_{i_{\text{Model}}}| + |HHV_{\max} - HHV_{i_{\text{Model}}}| + |A_{\min} - A_{i_{\text{Model}}}| + |B_{\min} - B_{i_{\text{Model}}}| + |C_{\min} - C_{i_{\text{Model}}}| + |D_{\min} - D_{i_{\text{Model}}}| + |E_{\min} - E_{i_{\text{Model}}}| \quad (5)$$

The process of minimizing the objective function J_i for each individual “ i ” involves using input parameters to calculate outputs based on the predictive models obtained from Weka, and an Excel program to evaluate the absolute errors. As the optimization method proceeds, individuals are evaluated by the objective function, and those best adapted are selected for the subsequent generation. This selection is random but proportional to each individual's performance against the objective function, allowing better-adapted individuals to be chosen more frequently. The crossover process then combines the selected parents to form the next generation. Various crossover methods, including one-point and two-point crossovers, are used to improve the algorithm's convergence. After crossover, random mutations ensure exploration of the search space. The mutation probability is critical. It can be manually set or calculated using an expression from Schaffer et al., based on experimental results to estimate the optimal value. Once the new population has been formed, it must be reduced to match the original population size. This reduction can be simple or elitist, depending on whether the selection is from the descendants alone or from both the parents and descendants based on their fitness. The algorithm has converged when at least 95 % of the population shares the same value for a gene. The stopping criterion used dictates convergence when a certain percentage of the population's individuals have converged. For successive optimizations, an initial population is generated within the studied range of values for each database. After evaluating the initial individuals, parent selection, crossover with a particular mask, and mutation follow, with the reduction set as elitist and a stopping criterion at 98 % similarity of the best value to the generation's mean. Once the best model for each variable has been obtained, the configuration is extracted to enable its automatic use in the genetic method, thereby facilitating the generation of predictions.

2.7. Life cycle assessment method

The International Organization for Standardization Standard (ISO) 14040/14044 [45] was followed in the life cycle assessment of this biodiesel production process. The LCA approach consists of four phases. These include (i) defining the goal and scope, (ii) conducting a life cycle inventory, (iii) assessing the impact of the life cycle, and (iv) interpreting the results. The manufacture of 1 kg of biodiesel from used cooking oil was chosen as the functional unit to specify the goal of this investigation. This biodiesel production process system boundaries are limited to a “gate-to-gate” method. This method determines the elements that probably have an impact on the environment using scaled-up inventory data. Using sodium hydroxide as the catalyst for the transesterification process takes into account the midpoint indications in the manufacture of biodiesel quantitatively.

The first step in LCA method is crucial since the technique used for the subsequent steps will rely on the study's goals [46]. In the second step, it is necessary to collect all system inputs and outputs. In an LCA

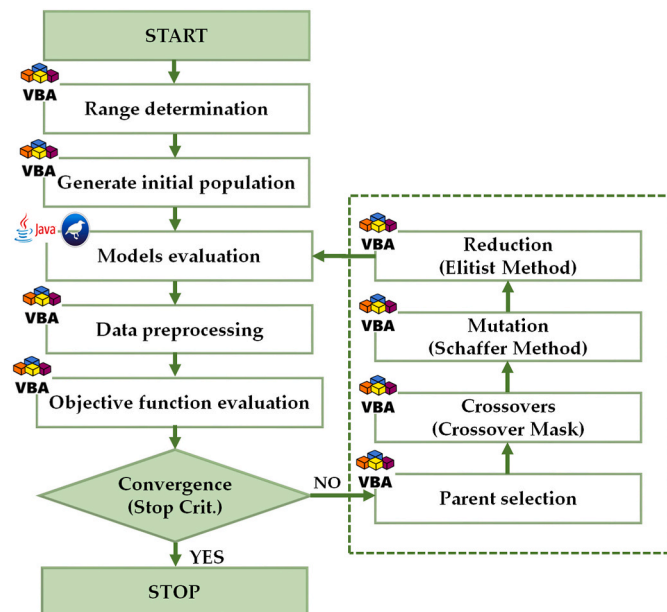


Fig. 2. Optimization with Genetic Algorithms workflow.

Table 3
Results for the errors in η and HHV in AddRegression model.

	Train			Test		
	Corr	MAE	RSME	Corr	MAE	RSME
η	0.995	0.008	0.024	0.986	0.007	0.023
HHV	0.807	0.097	0.123	0.787	0.098	0.134

Table 4

Obtaining a higher yield and heating value of biodiesel, while minimizing power consumption.

Var.	Goal	Min.	Max.	Optimum
A	Min	6.00	9.00	6.90
B	Min	1.00	2.00	1.00
C	Min	20.00	40.00	20.00
D	Min	500.00	1000.00	500.10
E	Min	20.00	40.00	30.00
η	Max	0.00	100.00	97.76
HHV	Max	0.00	45.06	43.19
Generation				12

study, this is the most costly and time-consuming step. Foreground and background data are the two types of data that typically should be listed in this step. According to Kiehbardrounizhad et al. (2023) [31], foreground data relates to the kind and quantity of all of the system's inputs and outputs. However, Background data is typically gathered from reliable databases. It is also connected to the environmental effects of the system's material and energy production and transportation. Background information for this investigation was sourced from the EcoInvent 3 database, which comprises life cycle inventory data covering all economic activities associated with various human activities. It is a consistent and coherent database [47]. For the third step of evaluating life cycle impact, several baselines may be used in accordance with the goals of the research. Due to its goal, midpoint and endpoint indicators have been used in the current work. For the midpoint indicator, the CML-IA database was used, whereas ReCiPe was used for the endpoint indicator. The midpoint indicators focus on specific environmental issues, such as abiotic depletion, ozone layer depletion, or global warming. However endpoint indicators have an environmental impact on three higher aggregate levels: human health, ecosystems, and resources. Understanding of the LCA data is made easier by converting midpoints to endpoints.

3. Results and discussion

3.1. Experimental results, model evaluation and selection

After completing the thirty-three transesterification processes according to the DoE design matrix, outputs process variables were established in the laboratory. These results appear in Table 2. The dataset was processed and assessed using WEKA, Version 3.9.5. As an open-source tool for machine learning, it facilitated the training, testing, and evaluation of the model's efficacy. Initially, a suite of machine learning algorithms was used for training using the dataset, that comprised input parameters and output variables gathered from laboratory experiments. WEKA software was used to create various prediction models for each of the input parameters that were analyzed. The determination of the best algorithms was based on their prediction errors. In this case, three key metrics were utilized: mean absolute error (MAE), root mean square error (RMSE), and the correlation coefficient (Corr). Among these models, Additive Regression (AR) was identified as the most effective model, it produced the fewest prediction errors for the output variables of yield and HHV. AR operates as a non-parametric regression technique that models the dependent variable as an aggregate of smooth functions of each independent variable [48]. This non-parametric approach does not assume a specific functional form for the relationship between the dependent and independent variables. This provides greater flexibility in capturing complex, non-linear interactions [49]. Each function represents the effect of a single independent variable. This enables the model to adapt to various shapes and forms, depending on the underlying data structure. A notable feature of AR is its ability to handle high-dimensional data while maintaining interpretability. This enables each component of the model to be examined

individually. This approach is particularly useful in scenarios where understanding the individual effects of predictors is as important as the predictive accuracy of the model. Parameters selected for applying AR in this study were as follows: batch size—100, classifier—bagging, shrinkage—1, and the number of iterations—30.

The most efficient model performance (AR) was determined by its higher Corr value (close to one) while minimizing the MAE and RMSE values (close zero). Table 3 displays the Corr, RMSE, and MAE. The Corr values are notably close to "1", indicating a strong correlation between the experimental observations and the predictions made by the Additive Regression (AR) models. Specifically, the yield showed the highest correlation (Corr = 0.9957), while the Higher Heating Value (HHV) had the lowest correlation (Corr = 0.8073). The low values of MAE and RMSE for the analyzed variables indicate that the regression models align closely with the experimental results. This demonstrates their accurate fitting and strong generalization ability. In this case, the yield (η) reveals the lowest MAE and RMSE for training and testing, respectively (MAE = 0.008 and RMSE = 0.024; MAE = 0.007 and RMSE = 0.023), while the higher heating value (HHV) has the highest MAE and RMSE for training and testing, respectively (MAE = 0.097 and RMSE = 0.123; MAE = 0.098 and RMSE = 0.134). Similar results were obtained by other researchers using different regression models to predict η and HHV. For example, Daniyan et al. [50] proposed an ANN to predict η in the production of biodiesel from frying oil using the same process parameters. With a Central Composite Design (CCD) involving 15 experiments, the values obtained for Corr., MAE, and RMSE were, respectively for training: 0.9972, 0.36, and 1.83. Similarly, Mustapha et al. [51] used multi-response surface methodology (MRS) to determine the HHV from a mixture of various non-edible vegetable oils using the same process parameters. In this case, using a second-order polynomial model with 9 experiments, the values obtained for Corr., MAE, and RMSE were, respectively for training: 0.97, 0.310, and 0.398.

3.2. GA optimization

After the machine learning-driven regression models were selected, Genetic Algorithm (GA) was employed to fine-tune the parameters that were involved in the biodiesel production process. In this case, the algorithm that exhibited the strongest capability for generalization (AR) was employed to identify the optimal values of the parameters in the biodiesel manufacturing process. Table 4 shows a combination of the five input parameters that were studied for achieving optimal biodiesel production using GA. This approach aimed to maximize yield and HHV, while also reducing catalyst usage, the methanol-to-oil molar ratio, and energy consumption during production (minimizing reaction temperature, reaction time, and speed). The columns of Table 4 displays the input process parameters and the responses in this transesterification process optimization, the objective (minimum, within a specified range, and maximum), the minimum and maximum values within the biodiesel production range, and the optimized values. The optimal values for the transesterification process includes the catalyst dose (A), methanol-to-oil molar ratio (B), reaction temperature (C), reaction time (D), and stirring speed (E). The latter were identified as 1 wt%, 6.9 mg/L, 30 °C, 20 s, and 500.1 rpm respectively. The Generation indicates the number of iterations that, in this case, was 12, to arrive at these optimized values.

To confirm the optimal conditions, an experiment was conducted under this specific circumstances. This experimental validation yielded a 97.8 % success rate in biodiesel production. This confirmed that the predicted optimal conditions were appropriate. The results showed a Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) of 1.698 each, indicating a close match with the experimental data.

3.3. Life cycle assessment in biodiesel production

3.3.1. Goal and scope definition

The definition of the goal and scope is the first step in the life cycle assessment method. Therefore, it is necessary to clearly define these two matters. The main goal of this research is to employ the LCA method as a tool for evaluating and assessing the environmental burden of biodiesel. The production of 1 kg of biodiesel from waste cooking oil was the functional unit that was chosen to specify the desired result of this research. NaOH was selected as the transesterification catalyst for this biodiesel production procedure, and RSM determined the optimum process parameters: catalyst dose (A) = 1 wt%, methanol-to-oil molar ratio (B) = 6.9 mg/L, reaction temperature (C) = 30 °C, reaction time (D) = 20 s, and stirring speed (E) = 500.1 rpm.

The scope of the LCA in the production of biodiesel from waste cooking oil has been “gate-to-gate”. This means that the boundaries of this method included each input parameters of the transesterification process. However, the waste cooking oil transportation was not considered. As a result, the power used (W) by the magnetic hot stirrer, the reagents (methanol and sodium hydroxide), and the use of deionized water to eliminate residues of alcohol were taken into consideration in the life cycle assessment (LCA) approach in the present research. Although the amount of electricity (W) used to wash the biodiesel matched that of a low-voltage electrical source, the deionized water used was equivalent to natural water.

3.3.2. Midpoint indicator impact assessment

Simapro v.9.2.0.2 software was used to process the data and better comprehend the environmental impact. In this research and for midpoint indicator assessment, LCA was based on baseline CML-IA v3.06. This baseline approach for impact assessment limits the method to the first phases of the cause-and-effect chain. It offers simple handling and high transparency [52]. The Ecoinvent 3 database provided the inventory data for the inputs, whereas the process simulations provided the information on the material and energy utilized. This life cycle inventory includes all economic activities for various human activities that were involved in this biodiesel production process.

The midpoint indicator assessment revealed eleven categories of impacts on the environment, human health, and resources. These include eutrophication, acidification, global warming, ozone layer depletion, human toxicity, photochemical oxidation, abiotic depletion, abiotic depletion (fossil fuels), fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, and terrestrial ecotoxicity. The release of excessive nutrients leads to eutrophication. In the acidification, the size of the acidifying impact varies significantly based on the characteristics of the ecosystem exposed to acidifying substances. One of the primary environmental indicators is the global warming potential, which is determined by greenhouse gas emissions and is measured over a 100-year period [53]. Ozone layer depletion has a forty-year lifespan. Halides, a measure of human toxicity based on exposure to and interaction between the body and the hazardous substance, are the key factors influencing it. The release of active molecules that are detrimental to ecosystems and public health is known as photochemical oxidation. The unit of measurement for abiotic depletion is kilograms of antimony equivalent (kg Sb eq). It is in line with the exhaustion of fossil fuels. Fossil fuel extraction is associated with abiotic depletion (fossil fuels). The assessment of environmental toxicity in the biodiesel process takes into account the harm that is done to freshwater and groundwater sources, as well as the release of acidifying compounds into the environment [54]. Fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, and terrestrial ecotoxicity are the three main categories into which it is separated.

Table 5 and Fig. 3a show the results for the biodiesel production using waste cooking oil based on CML-IA baseline of midpoint indicator. Comparing these results with those of other researches, it can be seen that they are lower than those obtained for fossil diesel production [55].

Table 5

Impact category results for CML-IA baseline midpoint indicator assessment.

Impact category	Unit	Result
Abiotic depletion	kg Sb eq	8.447E-08
Abiotic depletion (fossil fuels)	MJ	12.876
Global warming (GWP100a)	kg CO ₂ eq	0.451
Ozone layer depletion	kg CFC-11 eq	4.05E-09
Human toxicity	kg 1,4-DB eq	0.136
Fresh water aquatic ecotoxicity	kg 1,4-DB eq	0.043
Marine aquatic ecotoxicity	kg 1,4-DB eq	159.002
Terrestrial ecotoxicity	kg 1,4-DB eq	1.531E-04
Photochemical oxidation	kg C ₂ H ₄ eq	1.412E-04
Acidification	kg SO ₂ eq	2.281E-03
Eutrophication	kg PO ₄ eq	6.537E-05

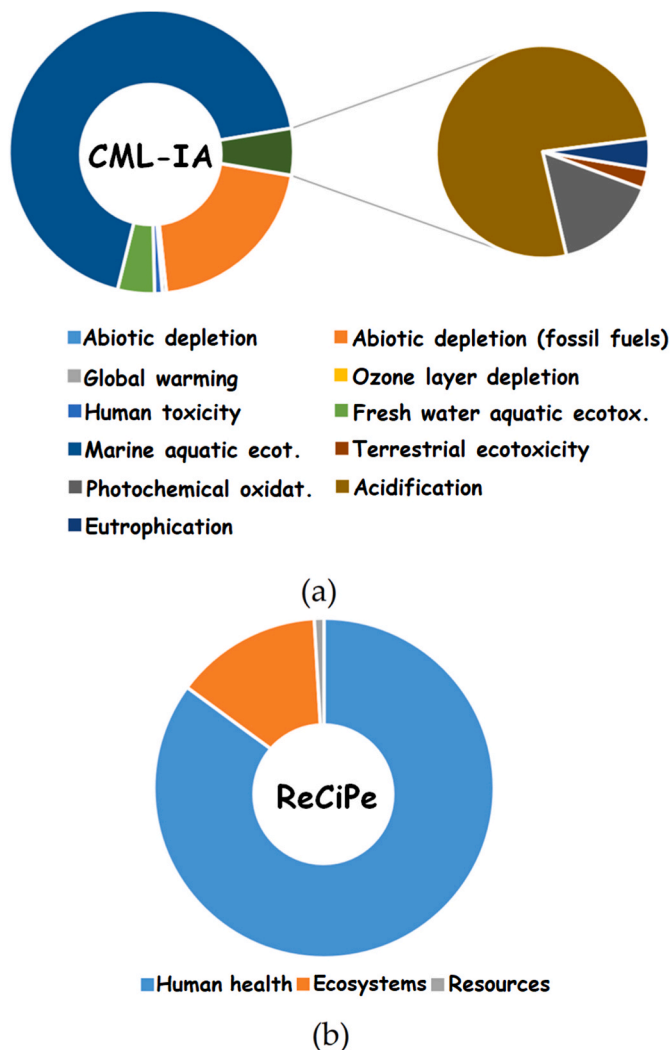


Fig. 3. (a) Normalized CML-IA baseline results diagram for midpoint indicator and (b) Normalized ReCiPe baseline results diagram for endpoint indicator.

The fact that sodium hydroxide, the catalyst utilized in this study, is less toxic than the ingredients used in the manufacturing of diesel, explains why the creation of WCO biodiesel was less dangerous. Furthermore, it is shown low environmental impacts since used cooking oil was gathered straight from restaurants and the calculations did not include agriculture or production stages. The same conclusion was obtained in the study of Chung et al. (2019) [56]. The environmental effect level for this biodiesel production process was found to be lower than that of other forms of biodiesel manufacturing. For example

Hosseinzadeh-Bandbafha used palm kernel shell-derived sulfonated magnetic biochar and obtained higher values of global warming, acidification, terrestrial ecotoxicity, or fresh water ecotoxicity [15].

3.3.3. Endpoint indicator impact assessment

In the current research, ReCiPe 2016 Endpoint (E) v1.03 was used for endpoint analysis. The endpoint indicator revealed three categories of impacts: (1) human health, (2) ecosystems, and (3) resources. In regard to human health, the number of illnesses linked to life years (measured in disability-adjusted life years (DALY)) rises as a result of environmental degradation. Acidification, ecotoxicity, eutrophication, and land utilization (measured in species * years) are examples of ecosystems. Resources directly affect the amount of raw materials used and the amount of energy consumed (represented in dollars).

The results of damage impact based on ReCiPe baseline endpoint indicator assessment are shown in Table 6.

A normalizing procedure was employed in order to compare the effect assessment of this damage categories. This was accomplished by multiplying previous results by a weighting factor. Because the weighted findings have the same units, they could be combined to yield a single environmental impact rating. As can be seen in Fig. 3b, the highest damage category value was human health, followed by ecosystems and resources. This might be as a result of using energy and catalyst in the transesterification process. It raised the volume of gasses that are hazardous to human health. However, this result is lower than those obtained in the study of [57]. Furthermore, when comparing the results with those obtained without the use of waste cooking oil [58], the same conclusion is reached as in the midpoint indicator assessment. The results are lower when waste cooking oil is used rather than being included in the production process.

3.4. Strength, weakness, opportunity and threat (SWOT)

The SWOT analysis is used to analyze development plans according to importance within a given industry [59]. It assesses methodically every possible angle or strategy, identifying obstacles and advantageous circumstances. The SWOT analysis concentrates on strengths, weaknesses, opportunities, and threats. An operational resolution may be aided efficiently by examining concurrently the qualities of internal and external systems. This is the main goal of a SWOT analysis. Depending on its origin, the SWOT analysis includes two categories, namely internal origin (strengths and weaknesses) and external origin (opportunities and threats) [60].

A SWOT analysis was conducted in this research in enhancing the efficiency and competitiveness of strategic planning for management of the waste cooking oil in biodiesel production. The analysis was undertaken to explore improved approaches for biodiesel production within the waste cooking oil value chains. This initiative not only contributes to refining strategic planning, but also to open opportunities to expand and enhance the value chains. In the context of biodiesel production from waste cooking oil, SWOT analysis serves as a valuable tool for strategic planning. Strengths encompass the advantageous features of the production process, while weaknesses highlight areas for improvement or limitation. Opportunities represent avenues for leveraging resources and capabilities, while threats denote potential challenges or risks to the project's success. This SWOT analysis for biodiesel production has been conducted, taking into account observations made during the production process itself, as well as insights gained through brainstorming

Table 6
Damage category results for ReCiPe baseline endpoint indicator assessment.

Damage category	Unit	Result
Human health	DALY	6.897E-06
Resources	USD2013	0.023
Ecosystems	species.yr	1.069E-08

sessions and relevant literature. For instance, the research of Liu et al. (2018) [61] aims to use SWOT analysis to assess the strengths, weaknesses, opportunities, and threats associated with waste cooking oil as a raw material for biodiesel production. Similarly, the study of Khan et al. (2021) [62] delves into various production and utilization aspects of biodiesel derived from waste cooking oil.

Table 7 illustrates the analysis, highlighting the advantages and potential challenges of implementing biodiesel production using waste cooking oil. This analysis aids comprehension of this process to achieve objectives and draws bring attention to areas that are overlooked or undeveloped.

4. Conclusions

This study focuses on multi-objective optimization utilizing Genetic Algorithms (GA) to identify the optimal set of input process parameters for sustainable biodiesel production. Artificial Intelligence (AI) techniques were applied to assess and optimize the effects of five critical factors in biodiesel production: catalyst dose (A), methanol-to-oil molar ratio (B), reaction temperature (C), reaction time (D), and stirring speed (E). The main output variables analyzed were the yield and HHV of the produced biodiesel. The results showed that under ideal conditions—specifically, a reaction temperature of 30 °C, a methanol tooil ratio of 1:6.9, a stirring speed of 500.1 rpm, a reaction time of 20 s, and a catalyst concentration of 1—the transesterification process achieved a maximum biodiesel yield of 97.764 %. This demonstrates the high accuracy of the optimized parameters, with a Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) closely matching the experimental results at 0.1678 and 0.1679, respectively. Additionally, a Life Cycle Assessment (LCA) was performed, utilizing both midpoint and endpoint indicators to evaluate the environmental impacts. This analysis concluded that the environmental footprint of this biodiesel production method is significantly lower compared to other biodiesel production techniques, highlighting its efficiency and sustainability. Additionally, a SWOT analysis was conducted to evaluate and enhance strategies for the biodiesel production value chains from used cooking oil. This analysis plays a vital role in identifying and capitalizing on potential opportunities to expand biofuel production value chains. By thoroughly examining the strengths, weaknesses, opportunities, and risks that are associated with these value chains, the analysis sheds light on the most effective ways to utilize used cooking oil for biodiesel production. This approach not only addresses the critical challenges of waste management. but also contributes significantly to a sustainable solution in meeting the growing demand for biofuels. The continual research and development in optimizing this process are essential and further solidify its feasibility as a sustainable approach. This aligns with the broader

Table 7
SWOT analysis for biodiesel production by waste cooking oil.

Strengths	Weaknesses
Use of recycled vegetable oils	Lack of raw materials due to high demand for biofuel
Does not interfere with other industries	Raw material instability
Contributes to the improvement of the environment	High initial investment
High quality and efficiency in the biodiesel obtained	High production cost
Opportunities	Threats
Growing need for the use of renewable energy	New competitors
High demand	Lower production than planned
Utilization of used oils	Lack of agreement with raw material suppliers
Supply of raw materials	Decrease in the price of oil
Lower environmental impact	Improved production of renewable energy in other industries
Replacement of fossil fuel	

global efforts to transition to renewable energy sources, highlighting the importance of sustainable practices in the biofuel industry. Future initiatives should prioritize conducting detailed energy analyses. The intention is to gain a thorough understanding of the sustainable production of biodiesel derived from different types of used oils. This should be achieved by leveraging advanced technological tools, which can provide deeper insights in the biodiesel production process.

CRediT authorship contribution statement

Marina Corral-Bobadilla: Writing – review & editing, Writing – original draft, Validation, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Rubén Lostado-Lorza:** Writing – review & editing, Validation, Data curation. **Celia Sabando-Fraile:** Writing – original draft, Investigation, Formal analysis, Data curation. **Saúl Íñiguez-Macedo:** Software.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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