

**ORIGINAL ARTICLE**

# Application of Supervised Machine Learning Models in Biodiesel Production Research - A Short Review

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**ABSTRACT** - Since industrialization, commercialization, and globalization of the supply chains in the world, non-renewable fossil fuels continue to be a primary source of energy for most of the segments. On the contrary, excessive consumption of these fuels has a significant impact on the environment and global ecosystem. Owing to several promising advantageous characteristics biodiesel fuels have attracted researchers and policy makers' attention as a replacement for non-renewable fossil diesels. There have been established biodiesel production experimental techniques focused on improving its yield and fuel characteristics. This short review focuses on covering supervised machine learning (SML) approaches in biodiesel production research. The SML methods powered predictions for biodiesel research not only optimizes the overall production process and fuel quality but also minimizes operational costs. The proposed analysis and directions will help prospective researchers in adopting machine learning to biodiesel research.

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**INTRODUCTION**

Over 80% of global energy needs are primarily provided by fossil sources including coal, petroleum, and natural gas indicates their essential part in development and heavy dependency on non-renewable sources [1]. Essentially the depleting fossil fuel reserves and increased utilization in industrial and transport sectors emitting greenhouse gases (GHG), causing climate change, global warming, air pollution, health problems [2]. In addition, Organization of the Petroleum Exporting Countries (OPEC) statistical reports projected world's demand for diesel and gas fuels in 2040 as 1834 billion liters which is about 10% more compared to 2017 usages [3; 4]. These critical developments directly pose significant challenges to the environment, ecological imbalance, and humanity. Owing to the energy crisis, the researchers, and policymakers' interests moved contributions towards clean and renewable alternative fuels such as biodiesel. With the growing trends by 2030 renewable fuel generated energy is expected to have a share of 23%. Compared to 2021, in 2022 it is expected that globally biofuel demand is anticipated as 6% or 9 100 million liters [5].

Biodiesel has been received as a sustainable choice due to advantageous physicochemical fuel properties and lower exhaust gas emissions, except nitrogen oxides. Although biodiesel has many benefits, the fuel suffers from stumbling limitations such as lower calorific values, higher viscosity, pour and cloud points, corrosion for large scale commercialization [6]. Biodiesel can be used in diesel-powered engines without significant changes [7]. Nevertheless, production and use of biodiesel and petro diesel blends are growing in both developed and developing countries including the USA, Germany, France, Malaysia, India, Brazil, Argentina, and Indonesia [5].

In addition to numerous experimental explorations, mathematical or statistical modeling techniques are widely used in biodiesel production and quality metric optimization. Traditional statistical data

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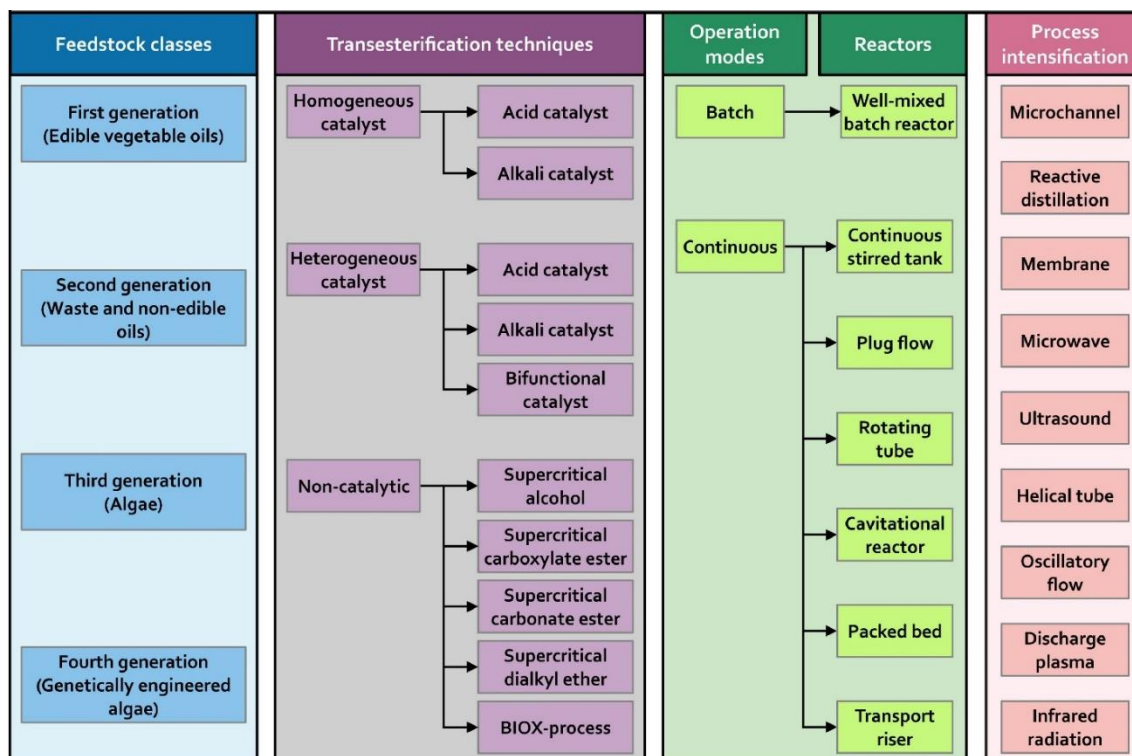
models are widely used in biodiesel production optimization research. Nonetheless, these approaches are constrained to capture intricate non-linear correlations of the biodiesel production as well as inadequate databases. Also, the predictive capabilities of these models are constrained in processing large datasets. Hence, it is essential to develop efficient, robust, and accurate mathematical modelling procedures for analyzing the correlations among various operating parameters and to optimize the desired outputs [8]. Further, a robust system estimation minimizes experiments within the set boundary conditions. In recent years there has been an efficient use of data-driven machine learning (ML) models in biodiesel production [9-11]. This short review paper presents basics of biodiesel production parametric studies, followed by state of use of machine learning algorithms in biodiesel research. Lastly concludes with applications of supervised machine learning (SML) algorithms, emphasizing on future perspective for adapting to the field of biodiesel production research.

### BIODIESEL FEEDSTOCK, PRODUCTION, AND QUALITY METRICS

Mathematically biodiesel production optimization is a multi-objective optimization problem (MOOP) [12; 13]. The objective functions concerned are complex and mutually depend on the competing constraints and parameters. The general form of MOOP is presented in Eq.1.

$$\begin{aligned}
 & \min/\max f_m(x), & m = 1,2, \dots, M \\
 & \text{Subject to } g_j(x) \geq 0, & j = 1,2, \dots, J \\
 & h_k(x) = 0, & k = 1,2, \dots, K \\
 & x_i^{(L)} \leq x_i \leq x_i^{(U)} & i = 1,2, \dots, n
 \end{aligned} \tag{1}$$

*L: Lower bound, U: Upper bound*

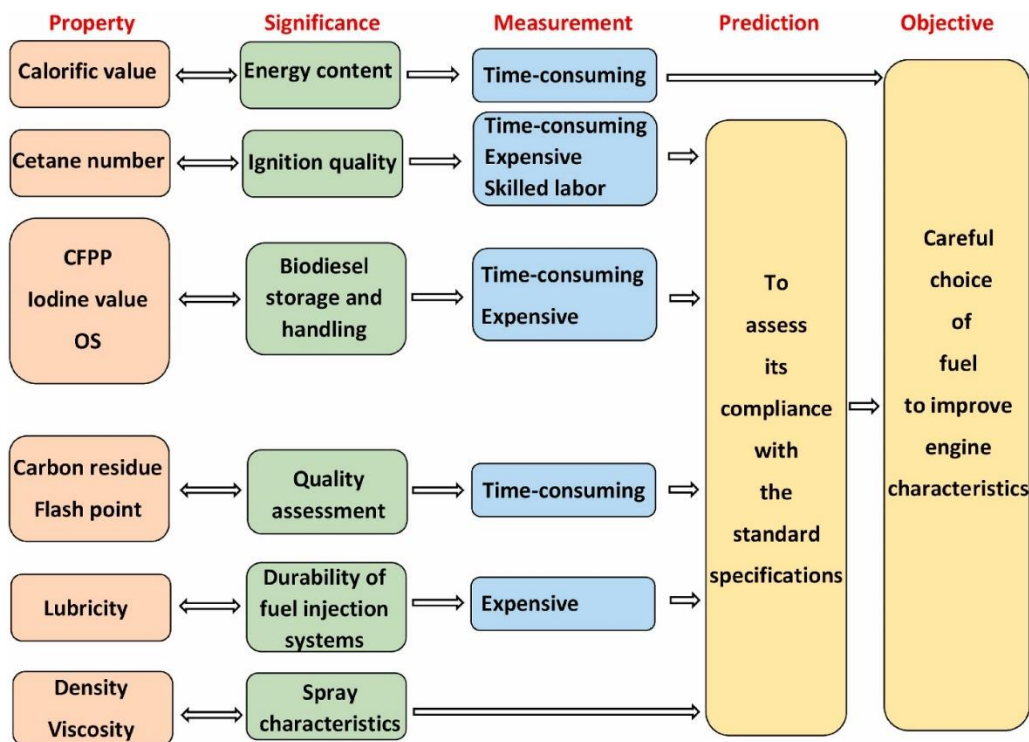


**Figure 1.** Classification of feedstock, techniques, reactors, and process intensification processes in biodiesel production [14; 15].

Classification and biodiesel production process influencing parameters are briefly presented in Figure 1. A wide range of promising feedstocks including edible non-edible vegetable oils, animal fat oils, waste

oils and microalgae can be used for producing biodiesels. The feedstock source characteristics such as geographical regions, seed genetic conditions, harvest season have significant effects on oil refining and purification processes [16]. However, use of edible oils has been strategically critiqued because of its estimated impact on oil prices. The feedstocks contain long-chain fatty acids that remarkably influence biodiesel process kinetics. Biodiesel is produced by esterification of free fatty acids (FFAs) or transesterification of triglycerides (TG) in the presence of a catalyst.

Researchers explored non-catalyst pathways of biodiesel production such as supercritical conditions [6]. Besides, biodiesel production involves a critical chemical procedure controlled by many parameters involving feedstock physicochemical properties, (trans)esterification process, alcohol type and quantity, catalyst type and concentration, reaction time, reaction and ambient temperatures, reactor geometry [17]. Consequent to the complexities in the biodiesel production mechanism substantially undertook sophisticated design and modeling methodologies. Numerical modeling of (trans)esterification reaction kinetics considering heat and mass transfer boundary conditions and subsequent simulations enhances biodiesel production processes [18]. Optimization of controlling and operating conditions results in produced biodiesel quality and quantity along with minimizing production cost, time, and flexibility in feedstock resources [8].

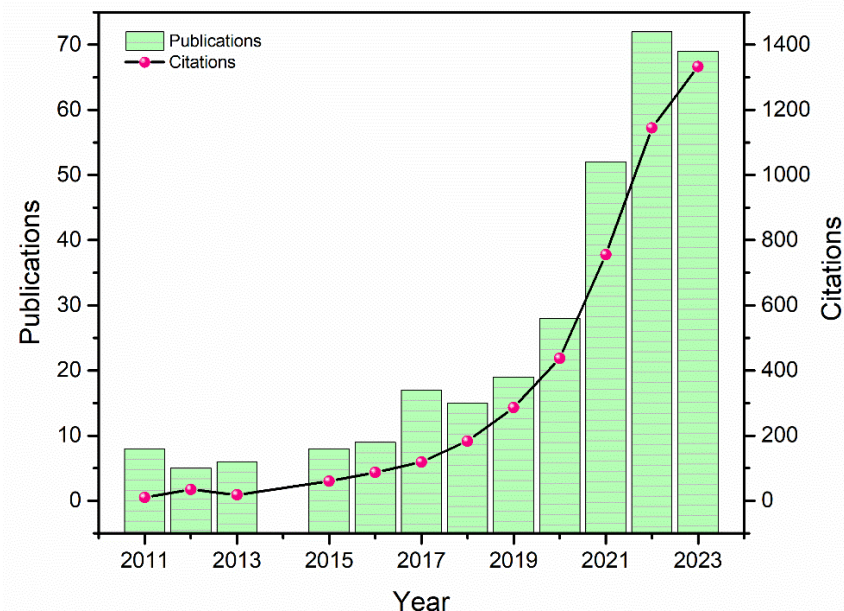


**Figure 2.** Importance of employing modeling techniques for predicting biodiesel fuel properties [19].

The biodiesel fuel properties determine its suitability for commercial application. European Norms (EN) and American Society for Testing and Materials (ASTM) standards determine fuel compliance. The important physicochemical property of a fuel includes density, viscosity, cetane number (CN), pour point (PP), cold point (CP), flash point (FP), cold filter plugging point (CFPP), oxidation stability (OS), iodine value (IV), acid value (AV) [16]. Many of these properties are potentially influenced by biodiesel feedstock, production process, storage, and transportation. Calibration, evaluation and optimization of the reaction kinetics of biodiesel production and its physicochemical properties require a comprehensive experimental data-driven analysis [19]. Importance of employing modeling techniques for predicting biodiesel fuel properties briefly resented in Figure 2. Statistical and mathematical models such as response surface methodologies are widely reported in optimizing including optimizing biodiesel production with limited datasets.

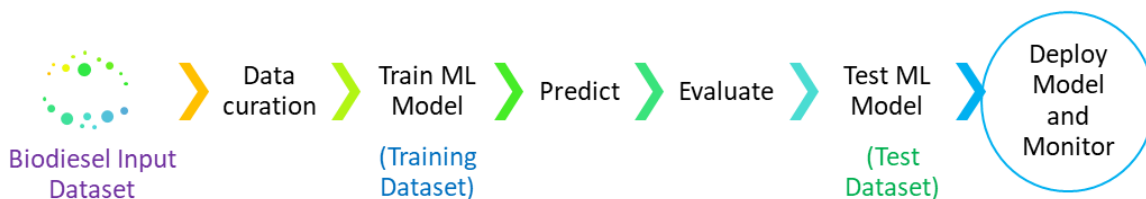
## MACHINE LEARNING TECHNOLOGIES IN BIODIESEL PRODUCTION RESEARCH

Machine learning model analytics in biodiesel production research can be applied considering numerous process domains including feedstock classification and supply chain, catalyst, production mode, controlling and operating parameters, and physicochemical fuel properties. Figure 3 shows recent data of research publications and citation details that employed ML models in biodiesel production.



**Figure 3.** Number of research publications that dealt with employing machine learning in biodiesel production research.

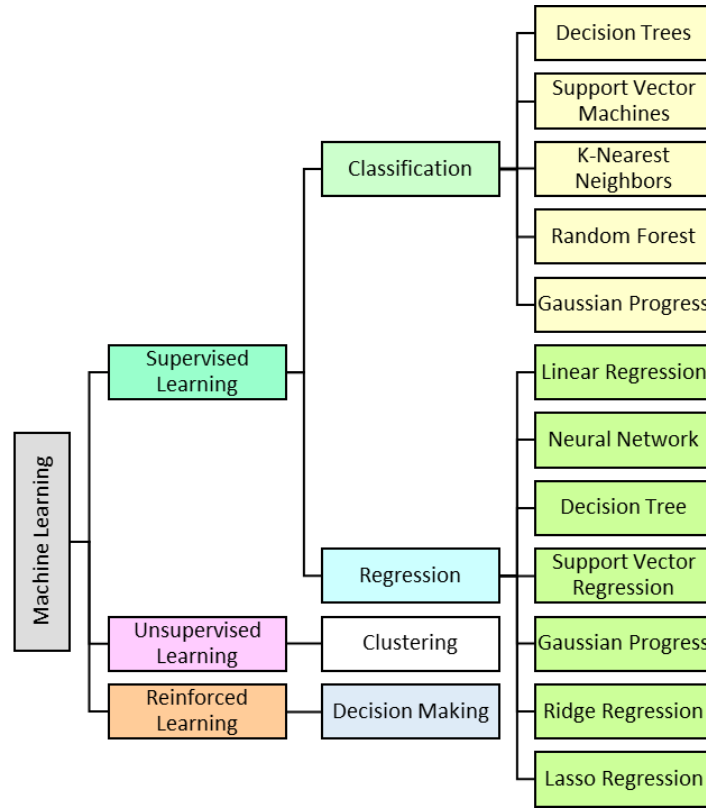
The ML programs are proven as a predictive analytics approach, that uses computational methods structured on algorithms for learning from input data sets and training to generate desired responses as output. The input parameters for a typical biodiesel production include catalyst concentration, methanol to oil ratio, reaction temperature, reaction time and agitation speed [20; 21]. While the output responses include biodiesel yield and fuel quality. Implementation of ML model workflow is presented in Figure 4. The Major steps include dataset collection, data curation, ML model training, Predicting the responses, evaluation, and testing of the ML model. Selection and adoption of a ML model broadly evolves on both the responses and tradeoffs of data sets and their complexity.



**Figure 4:** Machine learning model workflow for biodiesel data processing.

The comprehensive efforts made to review on ML models employed in biodiesel research reveals their potential applications in classification of biodiesel feedstock, biodiesel production, fuel property analysis, and biodiesel fueled diesel engine analytics [15; 20; 21; 22]. Among all ML models, supervised learning algorithms are being potentially devoted in various biodiesel production applications and there is a much scope for development.

**SUPERVISED MACHINE LEARNING MODELS IN BIODIESEL PRODUCTION RESEARCH.**



**Figure 5.** Broad categorization of supervised machine learning models.

A wide range of tailor-made ML models are employed for multiple discoveries and optimization. Classification of ML algorithms shown in Figure 5. Broadly supervised learning, unsupervised learning, and reinforced learning. Supervised machine learning (SML) is a subcategory of ML, where a model is trained on a labeled dataset to yield the required output. While the results of these predictive analysis are used to build applications such as feedstock studies, fuel quality prediction, yield estimation, production optimization, and process parameters. In biodiesel research, for classification and regression analysis ML models are widely used. The built SML model’s performance is being continuously evaluated to achieve desirable accuracy. Evaluation metrics that uses for cross validation of SML models include RMSE, R<sup>2</sup> and MAPE Eq. (2-4). However, based on ML models, other metrics such as F1 score, kolomogorov Smirnov chart, Gini coefficient, confusion matrix and log loss are also used [23-25].

$$\text{Root mean squared error (RMSE)} = \sqrt{\frac{\sum_{i=1}^N (\text{Predicted}_i - \text{Actual}_i)^2}{N}} \tag{2}$$

Where: *N* is the total number of observations.

$$R - \text{squared (R}^2\text{)} = 1 - \frac{\text{Mean squared error (model)}}{\text{Mean squared error (baseline)}} \tag{3}$$

$$\text{Mean absolute percent error (MAPE)} = \frac{1}{n} \sum_{i=1}^n \left| \frac{\text{Actual value}_i - \text{Forecast value}_i}{\text{Actual value}_i} \right| \tag{4}$$

Table 1 describes biodiesel yield optimization employing various SML models considering input parameters including catalyst quantity (CQ), agitation speed (AS), methanol to oil ratio (MOR), reaction temperature, reaction time and agitation speed. Jin et al., employed three ML models kNN, SVM and RF to predict biodiesel production considering input features such as biodiesel feedstock type, catalyst, reaction temperature, and reaction time with a total of 381 experimental data collected from 13 cases [26]. Bukkarapu et al., [27] applied ANN and SVM based Multilinear regression models to predict biodiesel properties. Gradient boosting ML model combined with Genetic algorithm (GA) were utilized to predict and optimize biodiesel production yield from waste cooking oil feedstock [28]. AdaBoost regression ML models were utilized to predict fuel properties including flash point, oxidation stability, density, and viscosity for biodiesel fuel application public vehicles considering various reaction operating parameters including agitation speed, fuel blend composition, reaction duration and temperature [29]. Hoang et al. conducted experimental analysis of pyrolysis oil and biodiesel oil blends for an application of natural gas enriched homogeneous charge compression-ignition engine [30]. Data modeling and analysis was carried out employing RF and SVR ML models. A combination of Gradient boosting ML, RSM and GA were effectively employed for predicting WCO biodiesel yield and fuel characteristics and their applications in CI engines [31]. DNN, LR, PR and kNN ML algorithm models are adopted to prediction and analysis of *Jatropha* biodiesel production via transesterification process [32]. Silitonga et al. studied microwave assisted *Ceiba pentandra* oil biodiesel synthesis employing extreme ML algorithm models and RSM for optimizing process conditions considering methanol/ oil ratio, catalyst concentration, reaction time and stirring speed [33]. Long et al. applied ML model techniques on semi-continuous algal cultivation for biodiesel production [34]. Therefor the research works concluded that employing SML model predictions gives accurate results.

**Table 1.** Supervised machine learning models applied for biodiesel production research.

Feedstock(s)	Model input parameters					Dataset size	ML Model	Reference
	CQ	MOR	Temp	Time	AS			
Castor oil	✓	✓	✓	✓		156	ANN	[35]
Castor oil	✓	✓	✓	✓	✓	156	Least square SVM	[36]
Castor oil	✓	✓	✓	✓		156	SVM, GA	[37]
Degummed waste cooking oil	✓	✓		✓	✓	27	ANN and RSM	[38]
Esterified soybean oil	✓	✓		✓		17	LR and ANN	[39]
Esterified <i>Ceiba pentandra</i> oil	✓	✓	✓	✓	✓	46	kernel- ELM and ANN	[40]
<i>Jatropha</i> -algae oil blend	✓	✓	✓	✓		29	ANN	[41]
Polanga oil	✓	✓	✓	✓	✓	26	ANN, GA	[42]
Sunflower oil	✓	✓	✓	✓		456	ANN and RSM	[43]
waste cooking oil	✓	✓	✓	✓	✓	29	ELM SVM and RSM	[44]
waste cooking oil#	✓	✓	✓	✓	✓	56	SVM	[45]
Waste olive oil	✓	✓	✓	✓		45	ANN	[46]

#water content and impurity also considered for modeling

## FUTURE PERSPECTIVES AND RECOMMENDATIONS

Biodiesel fuel production and physicochemical properties assessment relies on higher accuracy and predictability of a model. As discussed previously, biodiesel production is a complex process. There are numerous factors influencing the fuel yield and its characteristics. The traditional and other linear mathematical models are constrained with dataset processing approaches. Hence, there is a need for developing reliable and sophisticated models that accommodate non-linear relationships between

empirical research results and production operating parameters. Owing to their simplicity the SML models are preferred to overcome the poor predictability of traditional linear models. Developing generic ML integrated models for datasets from laboratory experiments, industry and synthetic sources would enhance the model accuracy driven analytics. The analytics will help to breakthrough many limitations in this domain as well as commercialize the research.

## CONCLUSION

Several supervised machine learning models are presented in literature to improve biodiesel production research specific to fuel quality and transesterification process are discussed. Major factors are given to standardize and perspectives for formulations based on multi objective optimization nature of biodiesel research. Credibility of data-driven models depends on size of the dataset as well as statistical validation approaches. The most important methodology for enhanced efficiency of predicted models in biodiesel research could be evolved from industrial scale research. Among reported literature limited efforts are devoted to building integrated models for biodiesel experimental research and industrial process results. Supervised machine learning powered empirical biodiesel processes will surely contribute to establish the most effective, inexpensive, and sustainable biodiesel supply chain as compared to the present.

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