

# Data-Driven Assessment Of Edible And Non-Edible Oil Suitability For Sustainable Biodiesel Production Using Machine Learning Classification Models

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## Abstract

Biodiesel has the potential to make transportation fuels more sustainable than traditional fossil fuels. In recent years alternate sustainable energy sources are gaining popularity because it can reduce emission of greenhouse gas than conventional fuels. Various feedstocks are being explored for biodiesel production including waste cooking oil which proves to be cost effective implementing waste valorization. Production of good quality biodiesel requires proper selection of raw oil feedstock. The suitability of raw oil for biodiesel production is critically influenced by its physicochemical characteristics. In this research, machine learning techniques such as K- nearest Neighbour (KNN), Support Vector Machine (SVM) and Random Forest (RF) are employed to find the suitability of the waste cooking oil for the production of Biodiesel from the properties of the raw oil. Based on the quality of the produced biodiesel the suitability is classified as not suitable, low, medium and highly suitable category. RF classifier is able to produce the classification accuracy of 99.15 % whereas, KNN and SVM classifier produced 97 % and 95.76% respectively. This research is significant in biodiesel production, which can considerably reduce the time, effort and resources by avoiding unnecessary processing of unsuitable oil. Predicting the suitability in advance supports more efficient, sustainable biodiesel production.

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## I. INTRODUCTION

In recent years, renewable fuels gained its popularity due to the limitations of non-renewable fossil fuels. These limitations include environmental contamination, short supply of petroleum products, rising petroleum product prices, growing energy demands worldwide, decreasing fossil fuel reserves, and greenhouse effects causing global warming [1]. Various approaches of renewable energy like wind energy, biofuels and geothermal energy paved way to address these challenges [2]. Biodiesel is one of the good alternatives for petrodiesel [3]. It is made from various oils, fats and greases. It also provides additional market values to animal fats and vegetable oils thereby decreasing the dependency of imported oil. It also serves as a renewable source of energy. Biodiesel helps in reducing the greenhouse gas emissions thereby considerably reduces the carbon footprint. Air pollution is reduced by the use of biodiesel [3].

Biodiesel is produced using edible, non-edible oils including waste cooking oil. A two - step process is followed in biodiesel production which involves esterification followed by transesterification [4]. The with acid catalyst, Free Fatty Acid (FFA) react with alcohol and forms fatty acid esters. The converted esters in this process are used in second step transesterification to produce biodiesel.

Aghbashlo et al. [5] published an extensive review of ML application in the various stages of biodiesel production. Kalogirou et.al [6] gives an overview of usage of neural networks in renewable energy applications. Using artificial neural network, the solar steam generating plant is modelled. Also, Wang et al. [7] worked with renewable energy such as solar and wind using machine and deep learning models. Furthermore, several studies have been published recently on the use of Artificial Neural Network (ANN) and Machine Learning (ML) approaches in renewable energy, gaining global recognition [8-11]. Many studies have employed ML approaches in predicting various properties related to biodiesel.

Artificial intelligence is used to predict waste cooking oil methyl esters [12] using ANN model. It is also analysed with yield of fatty acid methyl ester (FAME). The comparative study is made with Response Surface Methodology (RSM) and ANN [13]. Najafi et al. [14] studied modelling the FAME yield using the RSM, ANN, radial basis function neural network (RBFNN), and adaptive Neuro-fuzzy inference system (ANFIS) models. ANFIS models have also been used to predict other biodiesel properties such as

density, flash point, and cloud point, with superior performance compared to other models [15-21]. Corral Bobadilla et al. [22] applied the support vector machine (SVM) model with the linear, polynomial, and RBF kernels for predicting the viscosity, turbidity, density, and FAME yield while optimizing the reaction conditions using the genetic algorithm (GA).

Studies on AI algorithms in the biodiesel production process is done and various algorithms were analysed. Regression algorithms, Neural Network algorithms and ANFIS techniques are used for prediction of properties or feed stock of biodiesel [23]. The optimized conditions for transesterification process are implemented using bio inspired algorithms coati and Salp swarm optimization algorithm. When these optimized conditions are used in the production process the yield of 98.8% is achieved. The average  $R^2$  of 0.97 is obtained for experimental run conducted 27 times [24]. Microalgae oil is used as feedstock for biodiesel production. The optimization technique used is Bayesian optimization algorithm. The regression  $R^2$  value obtained is 0.96. The output parameter in this study is the quantity of biodiesel production [25]. Research has been carried out to optimize the feedstock there by reducing the production cost by yielding high quantity of biodiesel [26]. Various machine learning models have been adopted to get better yield of biodiesel. The features taken for training the model is catalyst ratio, temperature, methanol-to-oil ratio and reaction time. The output is yield of biodiesel. The yield achieved is 97.06% [27]. Various other predictive models have been developed to achieve high yield of biodiesel with transesterification of vegetable oils [28].

From the published literature it is evident that many researchers implemented machine learning and ANFIS techniques to predict the yield of biodiesel or FAME. However, predicting the quality of biodiesel is not yet explored. In this research, an attempt is made to classify the suitability of raw oil for the production of good quality oil based on the physicochemical properties of the oil. Consuming food prepared with Waste Cooking Oil (WCO) can lead to several health hazards. Prolonged consumption of cooking oil which is repeatedly heated can be a cause of hepatic dysfunction [29]. Similarly, consumption of such oil can increase blood pressure total cholesterol and vascular inflammation [30]. In addition, the improper disposal of WCO impose environmental impact. Hence, it is essential to recycle or repurpose WCO. The Sathyabama Institute of Science and Technology, Chennai, India is running a mess which provides food for approximately 12,000 people daily. Hence the WCO generated from the institution mess is also used for the study along with other non-edible and edible oils.

## II. Data collection and Exploratory Analysis

Both edible and non-edible oils such as Watermelon seed oil, Groundnut oil, Rice bran oil, Grape seed oil, Custard apple oil, Sapota oil, Papaya oil, Canola oil, Chicken fat, Beef tallow, Waste ghee, Alovera oil, Wheat germ oil, Palm oil, Sweet almond oil, Cucumber seed oil, Cotton seed oil, Pongamia oil, Madhuca indica oil, Prosopis juliflora oil, Neem oil, Simarouba glauca oil, Soapnut oil are collected from various sources. Similarly household generated WCO, Institution generated WCO, WCO from restaurants and sweet shops are also considered for the study. However, all type of raw oil may not be suitable for making biodiesel, and the collected oil needs to be evaluated for its properties. In this study, the physicochemical properties of raw oils such as FFA, density, viscosity, moisture content, and thermal properties are measured using standard laboratory test procedures as given in Table I. The raw oil properties thus measured are analysed using the regression plot as shown in figure 1. From the regression plot, the nature of data distribution, relation between the raw oil properties and its dependencies can be analysed.

Table I ASTM standards used for evaluating Physicochemical properties of raw oil

Parameters	ASTM standards
Density	ASTM D792
Kinematic viscosity	ASTM D445
Flash point	ASTM D93
Fire point	ASTM D93
Cloud point	ASTM D2500
Pour point	ASTM D2500

Moisture content	ASTM D2709
Acid value	ASTM D664
Calorific value	ASTM D480913

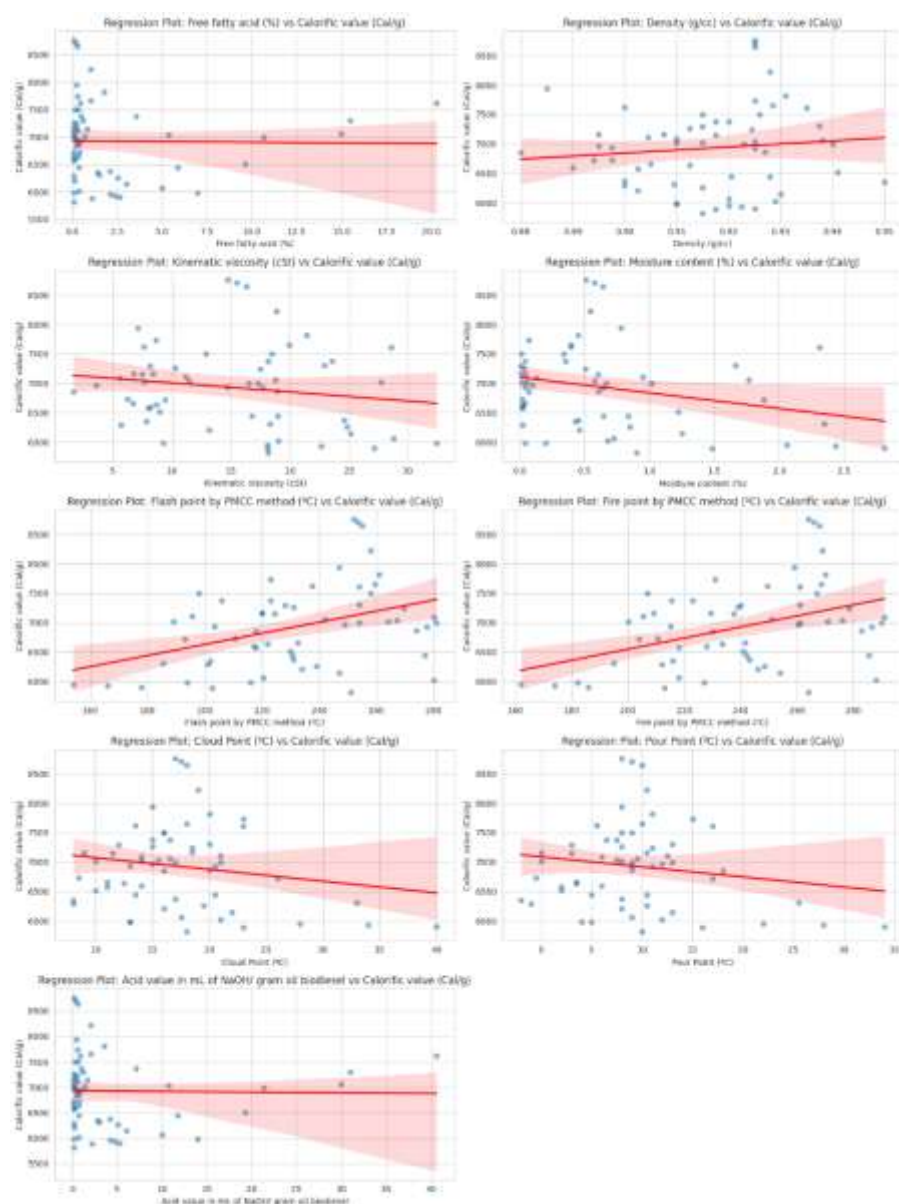


Figure 1 Regression plot for calorific value for various oil properties

Figure 1 shows the calorific values of raw oil for various raw oil properties. From the figure it is observed that the datapoints are scattered at low free fatty acid (FFA) value. The regression line is almost linear and flat which indicates higher FFA does not affect the calorific value. Since acid number and FFA has a direct relation, the trend with respect to acid number reflects similar relation. Density Vs calorific value shows slightly increasing trend, which implies the higher density oil will have slightly higher calorific value. Flash point and Fire point have a positive regression trend indicating higher the flash point and fire point higher would be the calorific value of the oil. Cloud point, pour point and moisture content shows slightly negative trend with calorific value which implies with higher values of these properties the calorific value will slightly decrease. The plot shows sparse distribution of data points and clustering within limited value ranges. With, uneven data distribution, the machine learning model may train to learn patterns dominated by densely populated regions. To address this issue, data augmentation is applied to

synthetically increase the dataset size without exceeding the original realistic range of each property as discussed in section III.

### III. Data Preparation and Augmentation

The prediction of biodiesel suitability using machine learning models relies heavily on the quality and quantity of input data. Raw oil from various sources is collected as discussed in previous section. However, collecting large volumes of experimental data depends on the availability of raw oil samples and the laboratory procedures. To address these issues and to enhance the robustness of the machine learning model data augmentation techniques were employed. Data augmentation prevents data overfitting and captures the variability of the raw oil properties.

In this study, two types of interpolation techniques are implemented for data augmentation namely linear and polynomial. To understand the relation between the physicochemical properties and the augmented data, Correlation Matrix is obtained with the interpolated data. Correlation matrix represents the degree of closeness or agreement between the raw oil properties. 1.00 value represents highest positive correlation among the two properties. -1.00 value represents the highest negative correlation among the two properties. Figure 2 and 3 shows the correlation matrix obtained for raw oil physicochemical properties with linear interpolated data and polynomial interpolated data respectively.

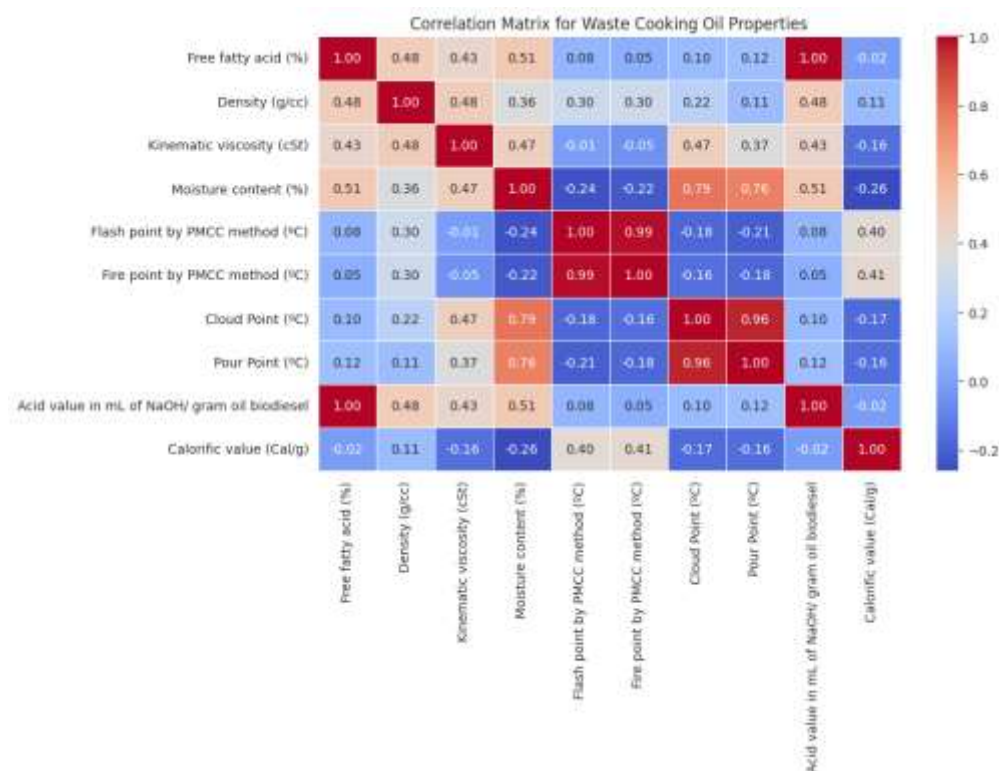


Figure 2 Correlation matrix for raw oil properties with linear interpolated data

From figure 2 it is observed that FFA and acid number has the highest positive correlation. Similarly flash and fire point has the high positive correlation (0.99) among them. Cloud point and pour point are having positive correlation with 0.96. Cloud and pour points are similarly correlated with moisture content with 0.79 and 0.76 respectively. Flash and fire points are moderately correlated with calorific value with 0.40 and 0.41 respectively. From figure 3 it is observed that FFA and acid number has the highest positive correlation. Similarly flash point and fire point has the highest positive correlation among them. Cloud point and pour point are having high positive correlation with 0.96. cloud and pour points are similarly correlated with moisture content with 0.81 and 0.82 respectively. Flash and fire points are moderately correlated with calorific value.

Upon comparing Figure 2 and 3, it is inferred that data augmentation with polynomial interpolation provided best correlation among the raw oil properties. Hence, the dataset used for this study comprise

of original data obtained by laboratory test procedure along with the data augmented using polynomial interpolation.

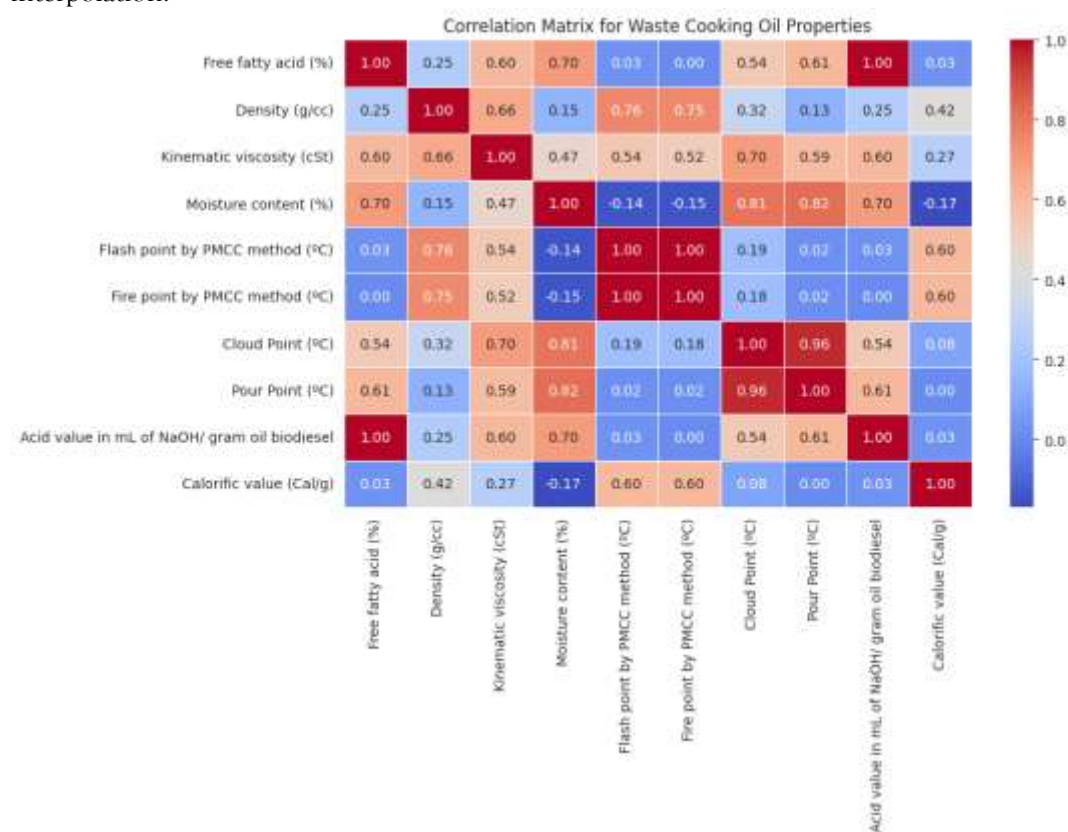


Figure 3 Correlation matrix for raw oil properties with polynomial interpolated data

#### IV. METHODOLOGY

The raw oil properties along with the augmented data through polynomial interpolation is fed to the Machine learning model. 4 target classes are considered, they are not suitable for biodiesel production, low, medium and high suitability for biodiesel production. In this research the supervisory learning algorithms such as support vector machine, K-Nearest neighbour and Random Forest are implemented for finding the suitability of raw oil for biodiesel production. In this section the detailed methodology of these algorithms is discussed as shown in Figure 4.

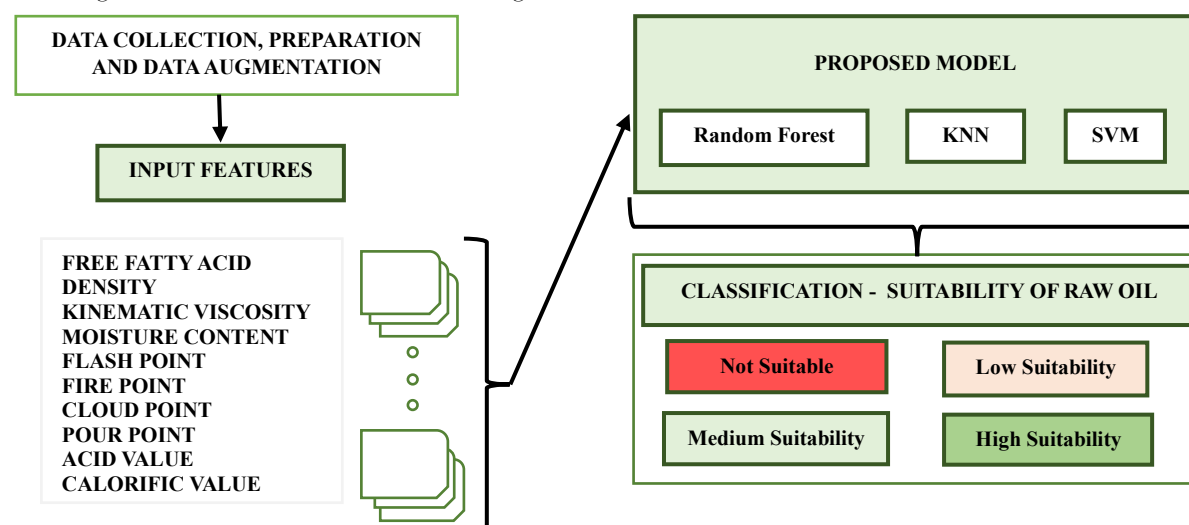


Figure 4 Schematic representation of the proposed system

**a) Multiclass SVM**

Multiclass-SVM is a supervisory learning algorithm which can be applied for both classification and regression tasks. This is a simple algorithm which separates the data based on the hyperplane in n-dimensional space corresponding to various classes. In this study 4 classes are used for finding the suitability of the raw oil for the biodiesel production. The output of the multiclass SVM can be computed using the input output relationship as given in equation (1)

$$y = mx + b \quad (1)$$

**b) K Nearest Neighbour (KNN)**

KNN algorithm classifies the unknown data based on the majority class of k nearest neighbours. The number of nearest neighbours depends on the k value assigned in the algorithm. In this study k value is considered as 5

The distance measure used for this study is Minkowski method as given in equation (2). The dataset is split into train and test set with 70 and 30 percent respectively. The performance of the algorithm is evaluated using k-fold cross validation method.

$$D(X, Y) = \left( \sum_{j=1}^n |x_j - y_j|^p \right)^{1/p} \quad (2)$$

Where, p is the order

$$X = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$$

$$Y = (y_1, y_2, \dots, y_n) \in \mathbb{R}^n$$

**c) Random Forest**

Random Forest is a powerful machine learning model that combines various decision trees. This algorithm is applied for reducing overfitting and improve the classification accuracy. The algorithm creates different decision trees with random subset, split from the training dataset. At each division, only a random selection of features is taken into account, which fosters diversity among trees. The Gini index is applied to measure the quality of a split in a decision tree as given in equation (3). Each decision tree produces a classification based on the features considered for the tree. The overall classification is decided based on the majority vote from all the decision trees as given in equation (4)

$$G = 1 - \sum_{i=1}^n p_i^2 \quad (3)$$

Where,

G - Gini Index

$$\hat{Y} = \text{mode}(\hat{Y}_1, \hat{Y}_2, \hat{Y}_3 \dots \dots \hat{Y}_i) \quad (4)$$

Where,

$\hat{Y}$  - Classification output

$\hat{Y}_i$  - Classification of  $i^{\text{th}}$  decision tree

**V. RESULT AND DISCUSSION**

The performance of the machine learning models can be analysed with the confusion matrix. The confusion matrix for the SVM, KNN and Random Forest classifier are shown in figure 5,6 and 7 respectively. From these figures it is clear that there is no misclassification for low and medium suitability class for all the algorithm. However, for high and not suitable class the misclassification is more. SVM separate the classes based on the optimal hyperplane. However, when the data distribution has overlaps between classes chance of misclassification is more with this classifier. Also, certain properties like Free fatty acid, Acid value, and Moisture content exhibit moderate correlations, which could lead to ambiguous separation when class boundaries are not defined sharply. KNN relies on distance metrics in the feature space. KNN tends to group the classes which has similar values for influential features. Whereas, Random Forest combines multiple decision trees, which reduces variance and overfitting making it robust to noisy features and outliers.

The performance of the models is analysed using the metrics such as sensitivity, specificity and accuracy as given by equation (5), (6), and (7) respectively. Table 2 shows the performance metrics of the classification models.



Figure 5 Confusion Matrix for SVM Classifier

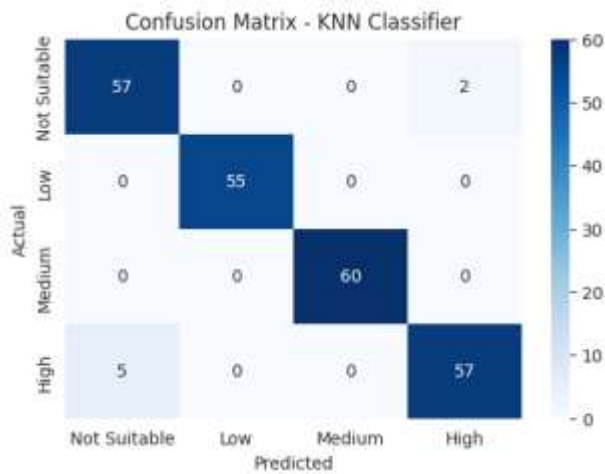


Figure 6 Confusion Matrix for KNN Classifier

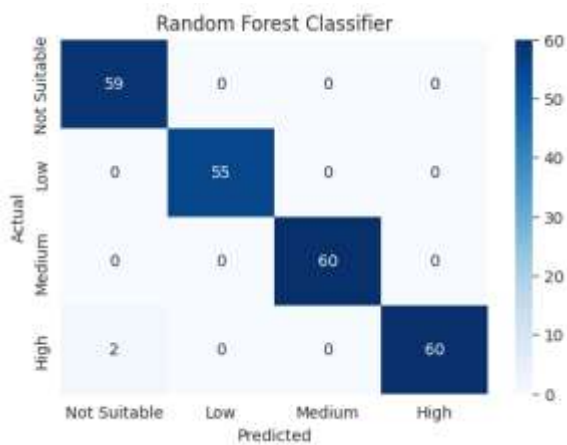


Figure 7 Confusion Matrix for Random Forest Classifier

$$Sensitivity = \frac{TP}{TP+FN} \quad (5)$$

$$Specificity = \frac{TN}{TN+FP} \quad (6)$$

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \quad (7)$$



Where,

TP - True positive which correctly identifies the specific class

TN - True negative which correctly identifies other corresponding classes

FP - False Positive which wrongly identifies other class as the specific class

FN - False Negative which wrongly identifies specific class as the other class

Table 2 Performance Analysis of Various Classifier

Methodology	Class	Sensitivity (%)	Specificity (%)	Accuracy per Class (%)	Overall Classification Accuracy (%)
SVM	Not Suitable	91.5	97.2	95.7	95.76
	Low	100	100	100	
	Medium	100	100	100	
	High	91.9	97.1	95.7	
KNN	Not Suitable	96.6	97.2	97.0	97.03
	Low	100	100	100	
	Medium	100	100	100	
	High	91.9	98.8	97.0	
Random Forest	Not Suitable	100	98.9	99.1	99.14
	Low	100	100	100	
	Medium	100	100	100	
	High	96.7	100	99.1	

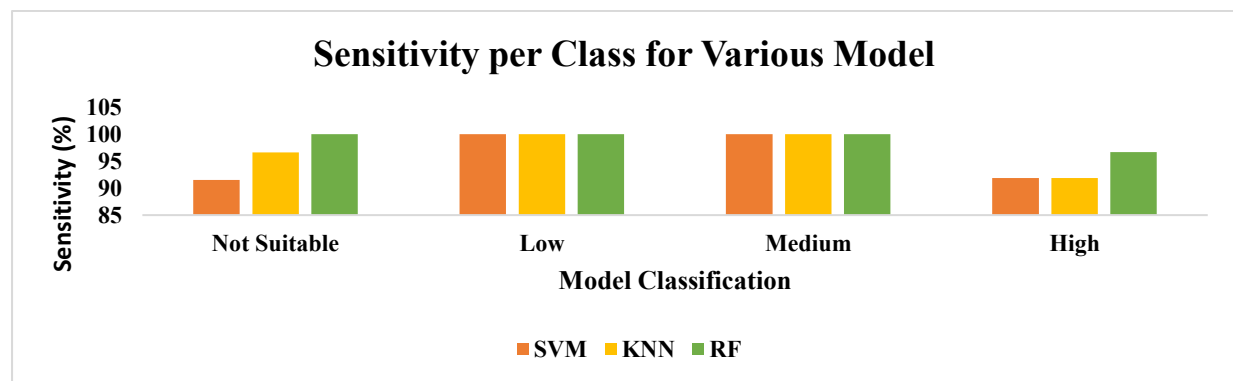


Figure 8 Performance of Sensitivity per Class for various classifier models

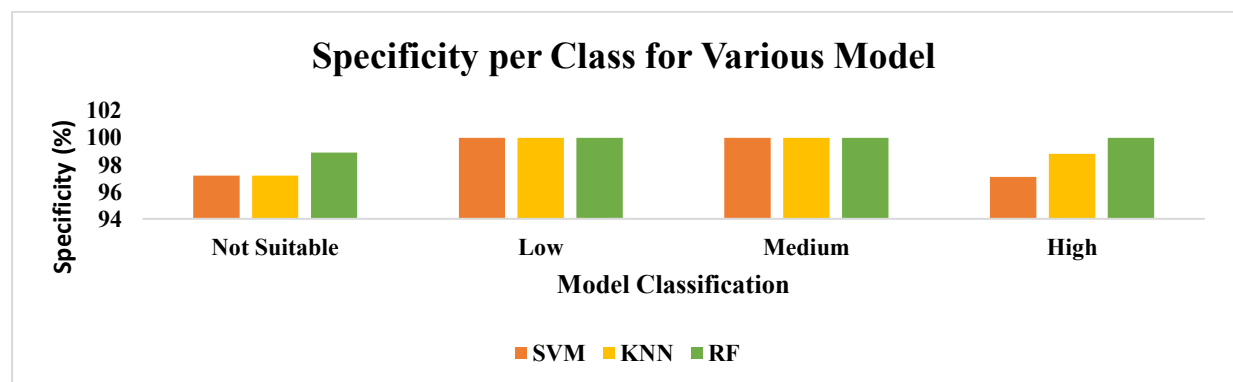


Figure 9 Performance of Specificity per Class for various classifier models



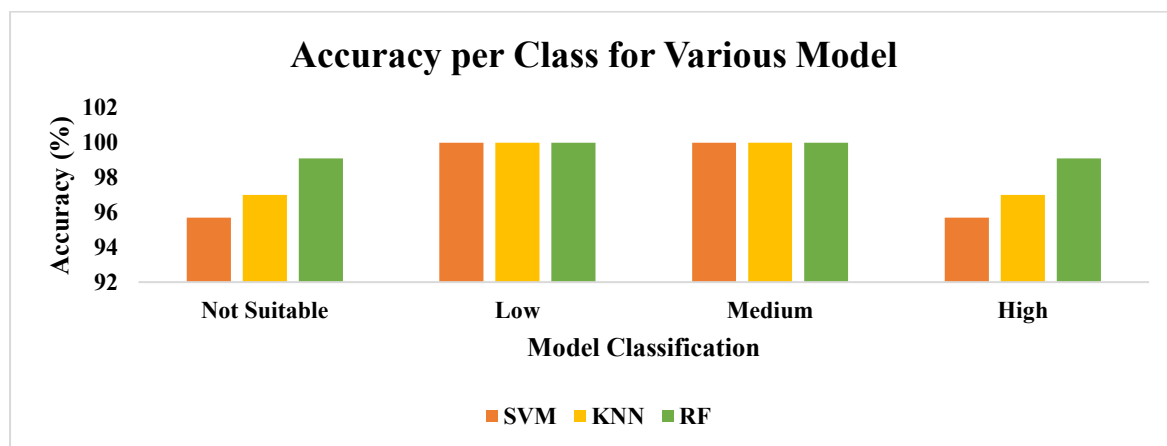


Figure 10 Performance of Accuracy per Class for various classifier models

From 8, 9 and 10 for all the classifiers 100 % performance is achieved with respect to sensitivity, specificity and accuracy per class for Low and Medium classes. Hence, it is inferred that these categories are well separated in the multidimensional feature space with respect to the oil properties. However, there is a challenge in accurately discriminating between High and Not Suitable categories. SVM and KNN classifier provided overall classification accuracy of 95.76 and 97.03 respectively. Whereas, Random Forest classifier provided overall classification accuracy of 99.14% which proves the suitability of ensemble learning in modeling complex and non-linear dataset. The results indicate that the selected oil properties are useful for assessing raw oil suitability for biodiesel production.

## VI. CONCLUSION

In this study, the suitability of various raw oils for biodiesel production is evaluated by analyzing various physicochemical properties. Due to the availability of limited dataset obtained through laboratory experiments, data augmentation techniques are applied to improve the dataset. Interdependencies between the physicochemical properties are analysed using correlation matrix and regression plots. The machine learning algorithms SVM, KNN and RF are trained to classify the oils into four suitability classes: Not Suitable, Low, Medium, and High. Random Forest classifier outperformed the other models by providing 99.14 % classification accuracy. This superior performance is due to ability of RF classifier to capture non-linear relationships and interactions between the oil properties. The research can be extended further for enhancing the prediction with larger dataset and more oil properties. Advanced deep learning techniques can also be explored for this study.

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