

Response Surface Methodology and Decision Tree Used in Oilseed Selection for Enhancing Biofuel Properties and Production in Cameroon

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Abstract

Oilseeds properties need to be improved for better biofuel production. In developing countries, oilseed plants remain the best and most affordable biomass used for industrial biofuel production. Indeed, industrial development of bio-fuels requires predictive modeling of the physicochemical properties of substrates and bio-oils produced during extraction. The main objective of this study was to predict physicochemical properties from three *Jatropha curcas* sp. seed samples. The jatropha seeds underwent determination of their lipid, cellulose, and dry matter content. The obtained bio-oils were characterized by their acidity, peroxide, and iodine values. Response surface methodology and a decision tree were used to predict the chemical properties of the bio-oils from the jatropha seeds samples. The results showed that kernel jatropha seeds had the lowest iodine and acidity values. There was no significant difference in iodine values between the jatropha seed samples. Using the response surface methodology, the optimal values for lipid, cellulose, and dry matter content were respectively 37.69%, 15.67%, and 96.65%, giving optimal bio-oil properties. For the Decision Tree, the physicochemical properties of the bio-oil from the three seed samples were predicted with a correlation coefficient of R^2 of 0.50, 0.9 and 0.4 corresponding to whole seed, kernel and crushed seed respectively. The model's robustness for Acid value, peroxide index and Iodine index shows a precision accuracy of 91%, 95% and 95% respectively. Predicting the physicochemical properties of oilseeds will be a major contribution to reducing operational costs and improving the efficiency of biofuel production mostly for developing countries.

Keywords

Jatropha curcas Oil, Prediction Efficiency, Iodine Index, Acid Index, Peroxide Index

1. Introduction

The development of biofuels in developing countries is obstructed by the global energy model's heavy reliance on fossil fuels [1]. Clearly, this model has been operating beyond its optimal capacity for a considerable period of time. The depletion of raw materials, the high extraction and production costs of fossil fuels, and the resulting greenhouse gas emissions and global warming have been identified as the main reasons for finding alternatives to fossil fuels [2] [3]. Furthermore, the utilization of fossil fuels indirectly escalates geopolitical tensions due to resource scarcity [4]. Confronted with these challenges, the international community has established sustainable development goals to mitigate climate change. The 2030 Sustainable Development Goals (SDGs) were established as guidelines for environmental protection. One component of the SDG 2030 initiative is reducing fossil fuel consumption [4]. To achieve this, we must pay particular attention to exploring alternative energy sources.

The global energy landscape is characterized by significant disparities in the distribution of energy resources. Despite the global expansion of biofuel production, there is still a need to explore the potential of biofuel sources further. Among these sources, biomass stands out as a reliable alternative energy source due to its renewability and relatively low production costs. In recent years, the importance of biomass fuels, more commonly referred to as biofuels, has increased significantly. Biofuels have the potential to serve as a primary energy source and contribute significantly to reducing global warming in the energy sector [5]. To achieve this, it is necessary to increase the production of bioethanol, biodiesel, and biogas and extend their use on a large scale, particularly in Africa. Numerous authors [6] [7] recommend the use of bioethanol and biodiesel based on technical and socio-economic factors. These factors include conventional production methods, integrating biofuels into existing transportation and supply networks, the acceptance of biofuels by local populations, and the availability of land for producing biofuel sources. To achieve this, it is crucial to consider the existing agricultural practices and methodologies used to produce and increase the productivity of biofuel sources, as they play a key role in ensuring a reliable and consistent biofuel supply [8].

Biofuels can be categorized into two main types based on the feedstocks used. First-generation biofuels are derived from food crops, such as sugarcane, corn, and soybeans. Second-generation biofuels are derived from non-food crops, such as switchgrass, algae, and agricultural waste [9]-[13]. Lignocellulosic biofuels, one of the feedstocks for second-generation biofuels, are considered an option for ad-

dressing high energy costs alongside increased energy efficiency and the use of alternative fuels [2]. Biodiesel, which is derived from oily plants such as oil palms and soybeans, as well as from unused cooking oil, is the second most common liquid biofuel after ethanol [10] [11]. Recent research has identified *Jatropha curcas*, a tropical oilseed plant, as a potential renewable fuel source with comparable energy content to diesel. Ref [12] [13] provide further insight into the oil content of *J. curcas*, which ranges from 40% to 60%.

Furthermore, three distinct types of *jatropha* seeds have been identified [13] [14]: whole seeds (*i.e.*, seeds in their original, intact form), kernels, and crushed seeds. Further ultimate and proximate analysis is necessary to determine the physicochemical properties of the various types of seeds, including their lipid, cellulose, and dry matter content. This is due to the presence of multiple growth conditions [11]. These properties will significantly impact the transesterification and biodiesel production processes. Laboratory analyses of the oil seeds can predict bio-oil characterization, which is advantageous for industrial purposes and agricultural decision-making.

Moreover, the literature shows that the optimization of lipid, cellulose, and dry matter content in oilseeds varies considerably, particularly in *jatropha* seeds. This complicates the selection of suitable seeds for oil production with optimal qualities for transesterification into biodiesel or direct energy use. This variability in physicochemical composition is primarily attributed to the geographic origin and cultivation location of the seeds. For example, [12] [15] characterized the physicochemical properties of *J. curcas* seed oil as having a lipid content of 59.32%, an acid index of 36.70%, and an iodine value of 104.90 mg/g. Ref [12] conducted a comparative analysis of two types of *jatropha* from two regions in Uganda. Their findings revealed significant differences in lipid content, free fatty acid levels, and acid index. Forecasting the characteristics of energy oils before extraction is crucial for improving the biofuel production process and reducing costs and time. Bio-oil obtained from *Jatropha* seeds can be characterized using simple, specific parameters requiring low-cost, rapid laboratory analysis [15]. Some of the parameters that could be used as bio-oil indicators include the iodine index, peroxide index, acid index, saponification index, and free fatty acid.

Many studies have been conducted in this regard, employing machine learning techniques [12]. The three-dimensional machine learning approach integrating RSM, ANN, and ANFIS models has been identified as a promising method for optimizing and modeling biodiesel production [15]. Additionally, using RSM in transesterification processes has been shown to make biodiesel more competitive with fossil fuels. Biodiesel production is affected by several variables, such as the methanol-to-oil ratio, catalyst ratio, temperature, and process duration. To predict the effect of these variables on biodiesel yield, various statistical techniques have been used [15]. Machine learning is the most widely used prediction technique for biodiesel production [16]. The optimal temperature was found to be 55°C; the ethanol-to-oil ratio, 35:1; and the catalyst amount, 15%, during *Jatropha*

oil conversion and fatty acid ethyl ester yield. Ref [17] investigated the optimization of yield and *Jatropha* biodiesel conversion through the implementation of RSM. The study identified an optimal yield of 96% and a conversion rate of 96%, with an optimal temperature of 60°C, a catalyst loading of 4 wt%, and a 6-hour reaction time.

As stated in previous research, most authors have focused on predicting and optimizing *jatropha* oil transesterification performance [17] [18]. However, this advanced research has only been applied in countries with well-established biofuel production processes. In Africa, and in Cameroon in particular, predicting bio-oil characterization before mechanical or chemical extraction is still underway. This progress must be undertaken with a comprehensive understanding of the physicochemical properties of the seed. In the context of *Jatropha*, predicting and optimizing bio-oil prior to extraction is essential for selecting the most suitable seeds for oil extraction based on physicochemical properties such as lipid, cellulose, and dry matter content. There is a lack of research in this area, and further investigation is required to establish optimal physicochemical property values for *Jatropha curcas* seed oil that can predict the quality of extracted bio-oil. Very few studies have investigated the statistical prediction of biodiesel based on the fatty acid composition of seed oils [18] [19]. This review lacks consideration of the optimization of bio-oil characteristics, such as iodine, peroxide, and acidity values derived from *Jatropha curcas* seed oil. Furthermore, the literature contains no discussion of optimizing *Jatropha curcas* oil seeds using decision trees and response surface methodology. This optimization will serve as an indicator for selecting the most appropriate seeds prior to mechanical or chemical extraction based on their physicochemical composition. Predicting this will reduce the energy and overall costs of the transesterification process by focusing only on high-quality oils. This approach will limit the ingredients required for intensive biodiesel production, as follows: Additionally, *Jatropha curcas* trees are experiencing the repercussions of climate change, resulting in a decline in the quantity and quality of production [20]. This phenomenon commonly occurs among oilseed crops in response to global environmental changes. Therefore, identifying the optimal physicochemical composition values related to lipids, cellulose, and dry matter is imperative to guide and control the agricultural production of these seeds, ensuring continuous productivity. This study's primary objective is to predict and optimize the bio-oil characteristics derived from *Jatropha curcas* seed oil using machine learning via RSM and decision tree approaches.

2. Materials and Methods

2.1. Acquisition of *Jatropha curcas* Seeds

Seeds were obtained from the Ndawara Farms Station in the Northwest region of Cameroon. For the current study, three samples of *Jatropha curcas* seed (whole seeds, kernels, and crushed seeds with hulls) were utilized (Figure 1). The hulling process involved removing the husks from the whole seeds to obtain the kernels.

An electrical grinder with a 0.005 mm sieve was used for the crushing process to produce crushed seeds. The three samples were then dried in an oven at a temperature range of 100°C - 105°C for 45 minutes, primarily to eliminate moisture content [19]. It was determined that all three samples had equivalent humidity levels (10%). For each seed sample, the lipid content (%), the cellulose content (%) and the dry matter content (%) were determined using the AOAC (2000) method.

The following section outlines the extraction process and the subsequent characterization of the oil.

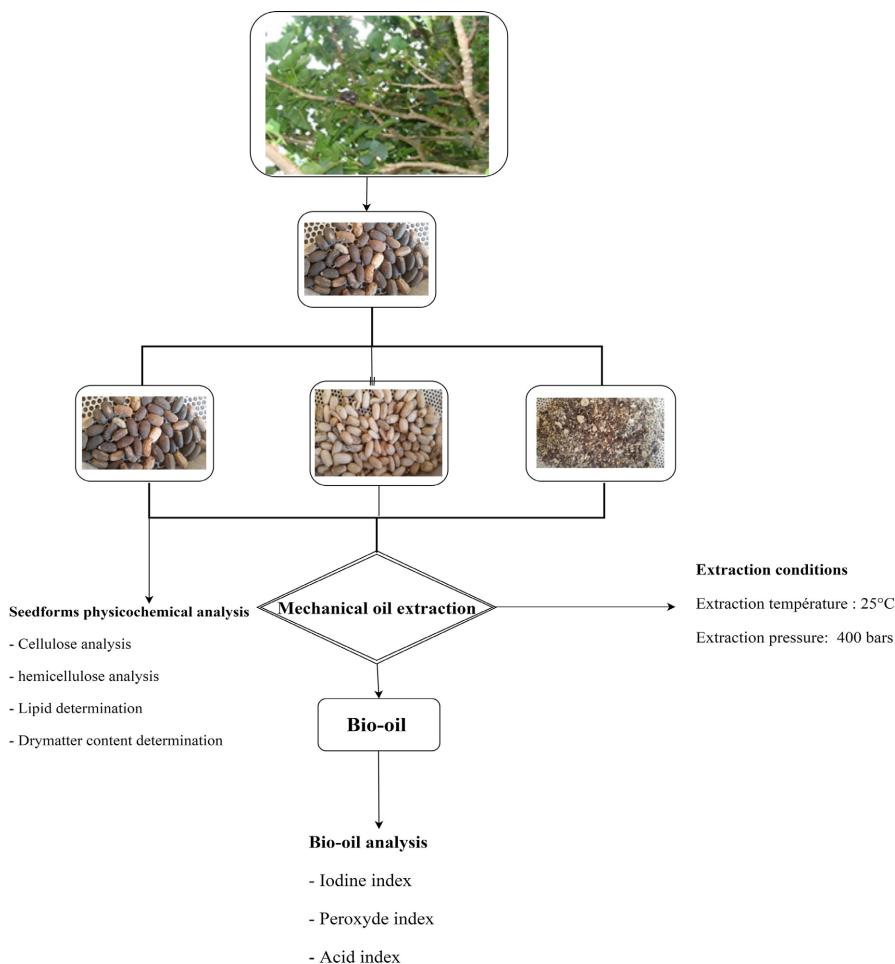


Figure 1. Flowchart of *Jatropha curcas* seedoil extraction.

2.2. Oil Extraction Process

Up to 6 kg for each dried *Jatropha* seed lots was placed in a mechanical extractor according to the method defined by [13] [14]. The collected oils were then analyzed in a laboratory to determine their iodine, peroxide, and acidity values. The oil extraction procedure was in three replicates.

2.3. Bio Oil Characterization

The acid, iodine, and peroxide values were determined using the standard method

established by ASTM D664 [18].

2.4. Prediction Methods

In this study, the prediction and optimization were carried out using the response surface methodology (RSM) and the decision tree. Note that the both machine learning technics are adapted to withstand small data sets while providing a good prediction performance in a system with nonlinear behavior [19] [20]. For the prediction process, three oilseed predictors were used, the lipid content (%), the cellulose content (%) and the dry matter content (%). As response variable as concerned, also 3 variables were chosen, the peroxide value (meq KOH/kg), iodine index (mg I₂/g oil), acidity index (%) applied to both RSM and decision tree.

2.4.1. Response Surface Methodology

In order to evaluate the three factors (lipids, cellulose and dry matter contents) that affect the three predictors (peroxide, iodine, and acid values) also known as responses, design of experiments (DOE) was used for the purpose. From [20], nonlinear relationship exists between the seed composition and the oil characteristics. With the above hypothesis, the response surface design was used to estimate any nonlinear interactions among factors. As shown in **Table 1**, 15 trials were generated for a Box-Behnken Design (BBD) in coded variables [−1, 0, +1], with lipid, cellulose, and dry matter serving as the independent variables, and iodine, acidity, and peroxide values serving as the responses. Note that the 15 runs were randomly simulated combinations. The simulation was done using measured data of dependent variables (iodine index, peroxide index and acid value). A code was designed and simulated in MATLAB 2015a to randomize the order of the runs, convert the coded design values to experimental values, and perform the experiment in the order specified. The response surface design was then used to estimate the nonlinear relationships between the contents of lipid, cellulose, and dry matter for each sample of *Jatropha* seeds.

Table 1. 3 factors Boxbenken Design applied to oil characteristics.

Number of experiments	Factors		
	Lipids (%)	Cellulose (%)	Drymatter (%)
8	−1	−1	0
14	−1	0	0
6	1	−1	0
1	1	1	0
7	−1	0	−1
9	−1	0	1
4	1	0	−1
2	1	0	1
11	0	−1	−1

Continued

13	0	-1	1
3	0	1	1
5	0	0	0
15	0	0	0
12	0	0	0

A series of experiments were carried out using the experimental data to determine the simulated data of lipid, cellulose, and dry matter content for each sample of *Jatropha* oilseeds.

2.4.2. Multiple Regression Models

In this study, the attributes representing lipid, cellulose, and dry matter content (see **Table 1**) were tested to determine their non-linear relationship with bio-oil properties. The polynomial function used for the multiple regression model is represented by Equation (1). The optimization process, using the Optimization Toolbox in MATLAB, determined the coefficients of the polynomial functions generated for each *jatropha* seed sample (whole, kernel, and crushed seeds). Equation (1) is presented below.

Quadratic model

$$= (\beta_1 \times L) + (\beta_2 \times C) + (\beta_3 \times DM) + (\beta_4 \times L \times C) + (\beta_5 \times L \times DM) + (\beta_6 \times C \times DM) + (\beta_7 \times L^2) + (\beta_8 \times C^2) + (\beta_9 \times DM^2) \quad (1)$$

L : Lipids (%); C : cellulose (%); DM : Drymatter (%)

Specifically, the coefficients $\beta_1, \beta_2, \beta_3, \dots, \beta_9$ of the quadratic equation were determined using a minimization/maximization function in Matlab. A code was written for this purpose.

2.4.3. Decision Tree

The main objective of the decision tree is to establish the relationship between each *Jatropha* seed sample composition (lipid, cellulose and dry matter) and the characteristics of the extracted oil (Iodine, Peroxyde and Acid values).

Table 2. Decision Tree input and output variables.

Variables	Types of variables	
	Input	Output
Jatropha seed sample	✓	
Iodine value		✓
Peroxide index		✓
		✓
Acid value		✓

As shown in **Table 2**, the *Jatropha* seed sample composition and the bio-oil characteristics were divided into input variable and output variable respectively. The decision tree predicted the iodine, peroxide, and acidity values of the oil based on the three *Jatropha* seed samples compositions (lipid, cellulose and dry matter contents). The threshold used to define quality classes was based on oil quality related to acid, iodine and peroxide values. **Table 3** shows the threshold values used for decision tree classification.

Table 3. Threshold classes for decision tree classification.

Classes	Biofuel quality		
	Low	High	Very high
Acid index (%)	>3.5	2.5 - 3.5	<2.5
Peroxide value (meq KOH/kg)	<19	19 - 24	>24
Iodine value (meq I ₂ /g oil)	<39	40 - 61	>62

To this end, the data were split into two subsets, training and test data. The split percentage was determined based on the models' ability to accurately predict the output variable without overfitting or underfitting the data [21]-[23]. **Table 4** presents the splitting percentage of the data set.

Table 4. Splitting percentage of the data set.

Data set type	Splitting percentage
	%
Training data	80
Test data	20

The decision tree uses training data to evaluate different attributes [22] [23] and was used to identify the best predictive parameters for bio-oil properties. This facilitated the establishment of the multiple regression model. The machine learning model was validated using test data. A Python script was used to determine the model's accuracy.

In order to mitigate overfitting, some key hyperparameters for tuning the decision tree model were designed and used in coding. The following are presented in **Table 5**.

Table 5. Decision tree model hyperparameter tuning.

Hyperparameters	Tuning value
Max Depth	5
Min samples split	15
Min samples leaf	15

Continued

Max features	sqrt
Criterion	Entropy
Tuning	Gridsearch, Randomsearch
Cross validation performance	85%

2.5. Model Performance Determination

Both R^2 and the root mean square error (RMSE) were used to evaluate the performance of both RSM and the Decision Tree. Equation (2) is the coefficient of correlation.

$$R^2 = 1 - \frac{\sum_{i=0}^N (y_i - \hat{y}_i)^2}{\sum_{i=0}^N (y_i - \bar{y}_i)^2} \quad (2)$$

The Equation (3) is the root mean square error.

$$RMSE^2 = \sqrt{\sum_{i=0}^N (y_i - \hat{y}_i)^2} \quad (3)$$

y_i : Dependant variable; $\hat{y}$: Predicted dependant variable; $\bar{y}_i$: Mean value of dependant variable.

Prediction accuracy was determined and applied only for the decision tree model.

2.6. Statistical Analysis

The Statistical analysis was conducted using python 2020. To compare mean value for the treatment (Seed sample comparison), the one factor anova test was carried out ($p < 0.05$).

3. Results and Discussion**3.1. Cellulose Content for Different Seed Forms**

The cellulose content of different forms of jatropha seeds is shown in **Figure 2**. It can be seen that whole and crushed seeds have the highest cellulose content ($p > 0.05$).

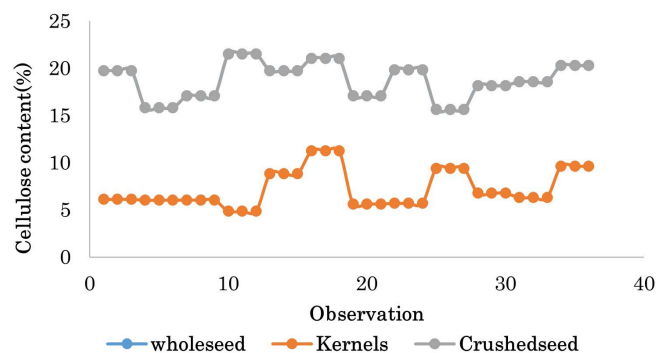


Figure 2. Cellulose content for different type of Jatropha seed oil.

The cellulose content was lowest in almonds ($p < 0.05$). Although they were taken from the same sample, there was a significant difference in cellulose content between whole seeds and almonds. Conversely, no significant difference was observed between whole and crushed seeds. This difference could be due to the presence of hulls in whole seeds and the absence of hulls in almonds. The presence of hulls could have led to an increase in cells, or cellulose building blocks. This differs from literature [20]-[24], which states that cellulose content does not vary within the same seed sample regardless of shape. However, the cellulose content values observed in this study are slightly different to those reported in the literature. In fact the seed maturity might be the main reason.

3.2. Lipid Content for Different Seed Forms

Figure 3 illustrates the lipid content of different *Jatropha* seeds. Kernels had the highest lipid content ($p < 0.05$). Whole and crushed seeds had the lowest values.

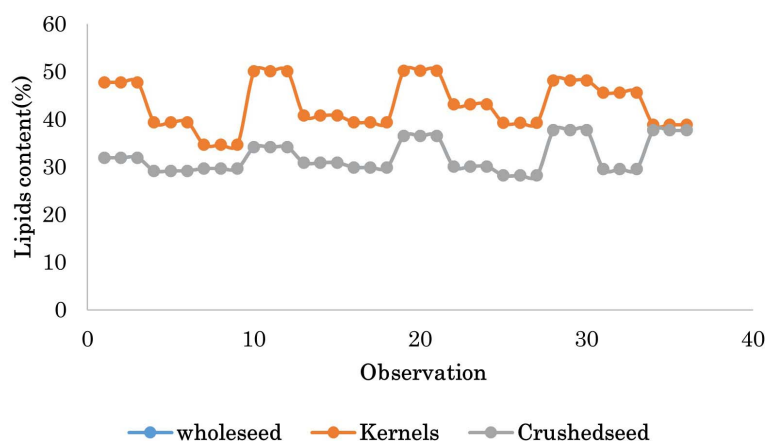


Figure 3. Lipid content for different type of *Jatropha* seed oil.

The lipid content in this study differs from that reported in the literature. One might think that production location and cultivation techniques are responsible for this variability. However, the variation in lipid content within the same grain sample could be likely due to the presence of hulls, which increase cellulose content and reduce lipid content [14].

3.3. Dry Matter Content for Different Seed Forms

Figure 4 illustrates the dry matter contents of the different forms of *jatropha* seeds. Irrespective of the form, dry matter contents were highest ($p < 0.05$) for whole seeds, followed by crushed seeds and kernels.

The significant difference in dry matter content between the seeds could be mainly due to weight differences related to the presence of hulls. The dry matter content values differ considerably from those reported in the literature review. The storage condition might be the main reason.

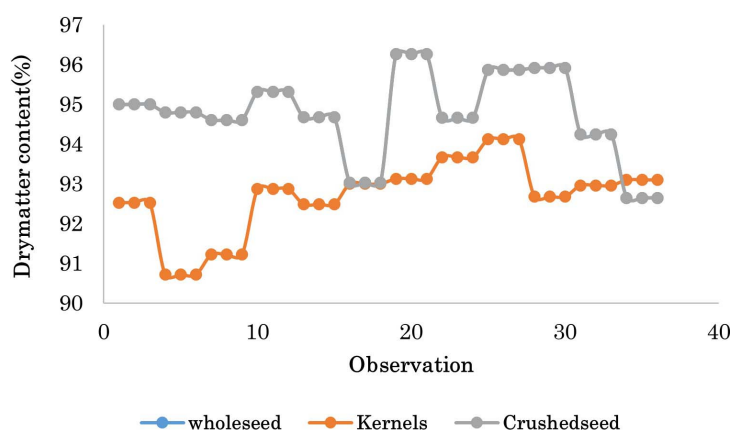


Figure 4. Dry matter for different type of *Jatropha* seed oil.

3.4. Characterization of Bio Oils Extracted from Different Groups of *Jatropha curcas* Seeds

3.4.1. Characterization of Iodine Value According to *Jatropha* Seed Type

Figure 5 shows the iodine value of the different seed forms. Regardless of the seed group, the highest iodine values were observed for bio-oils obtained from whole seeds, followed by those obtained from crushed seeds and kernels ($p > 0.05$). The iodine index actually measures the degree of oil saturation. The higher the iodine index, the less saturated the oil.

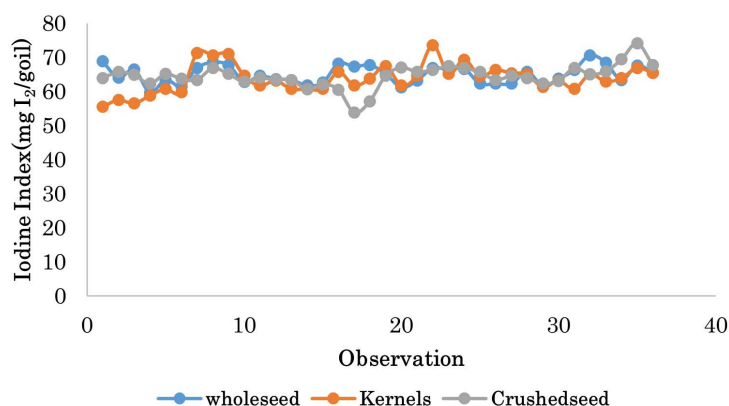


Figure 5. Iodine index for different type of *Jatropha* seed oil.

The iodine values of the bio-oil are slightly higher than [25] results and lower than those found by [17]. The iodine value of Cameroonian *Jatropha curcas* oil ranged from 62 to 66 mg I₂/g oil, which aligns with the EN14214 standard [25] [26]. Additionally, the one-way ANOVA model indicates no significant difference between the groups of seeds at $p < 0.05$. Therefore, the biodiesel produced from Cameroonian *Jatropha curcas* oil is ideal for engines. Remember that the lower the iodine value, the better the fuel will be as biodiesel.

3.4.2. Characterization of the Peroxide Value

Figure 6 shows the peroxide values of the *Jatropha* seed group. The peroxide index

measures the degree to which the oils degrade after extraction. The higher the index, the more degraded the oil [27]. The lowest peroxide value was obtained with the vegetable oil from the kernels, followed by the crushed seeds, then the whole seeds.

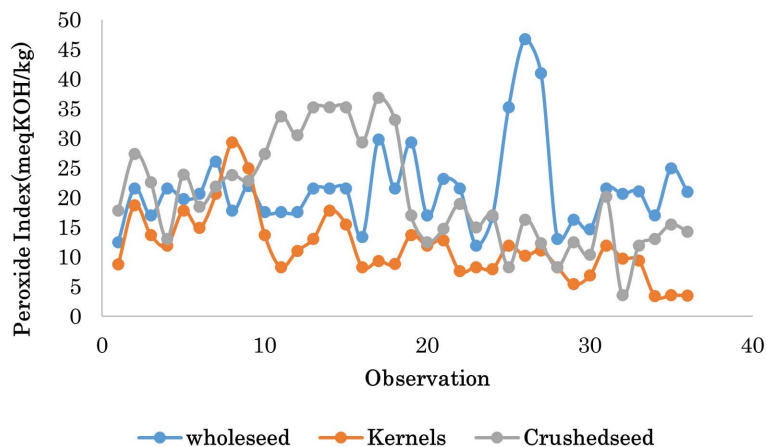


Figure 6. Peroxide index for different type of Jatropha seed oil.

The peroxide value varies significantly ($p = 1.6e-07$) among the seed form groups. The main difference between the groups may be related to the presence or absence of the seed oil's husk. Regardless of the seed group, the peroxide value of the Cameroon variety *Jatropha curcas* was between 10 and 24 meq KOH/kg. This value is relatively higher than those obtained by [28]-[25] for Nigerian and Ethiopian *Jatropha curcas* oils, respectively.

3.4.3. Characterization of Acid Index Based on Jatropha Seed Types

Figure 7 shows the acid value as a function of the seed oil group. The lowest acid value was obtained with oil from kernel seeds, followed by oil from whole and crushed seeds. The acid value indicates the type and amount of catalyst used in the transesterification process.

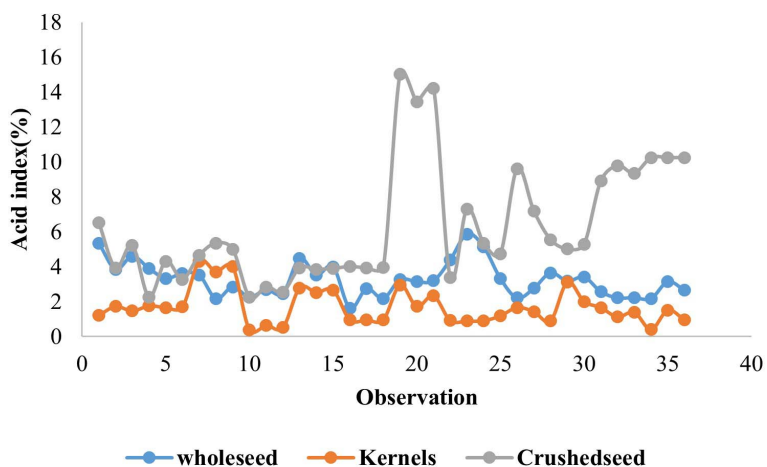


Figure 7. Acid index for different type of Jatropha seed oil.

There are significant differences between the seed groups. The main difference between the groups may be due to the presence or absence of husks on the seeds, which would reduce or increase the number of cells during oil extraction. This would result in lower or higher production of fatty acids and decreased or increased acidity in the oil. Regardless of the Cameroonian *Jatropha* seed group, the acidity ranged from 0% - 2% for kernels and 3% - 7% for whole seeds. These ranges are similar to those reported by [16] [29]. However, the higher acidity of oil from crushed seeds could be related to the small particle size during extraction.

3.5. Correlation between Seed Composition and Bio Oil

3.5.1. Iodine Index as Function of Lipids Content

Figure 8 illustrates the correlation between iodine value and lipid content. Regardless of the type of seed, the iodine value ranges from 10 to 70 milligrams of iodine per gram of oil. This demonstrates that the iodine value does not vary with lipid content among different types of seeds.

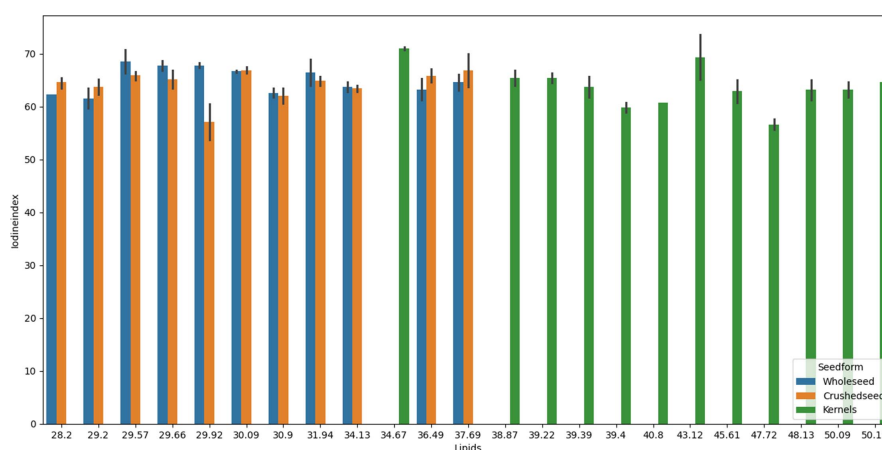


Figure 8. Iodine index as a function of lipid content of *jatropha* seed oil.

However, the highest iodine value was obtained with kernels at a lipid content of 34.67%. The lowest value was also observed with kernels, but at a fat content of 47.72%.

3.5.2. Iodine Index as Function of Cellulose Content

Figure 9 illustrates the relationship between iodine value and cellulose content. The iodine value varies little among different seed forms. However, kernels with a cellulose content of 6.06% had the highest iodine values. Conversely, the lowest iodine value was obtained in crushed seeds with a cellulose content of 21.06%.

Conversely, the lowest iodine value was obtained in crushed seeds with a cellulose content of 21.06%. There was no difference in iodine values between whole and crushed seeds, irrespective of the cellulose content.

3.5.3. Iodine Index as Function of Dry Matter Content

Figure 10 illustrates the relationship between iodine value and dry matter content.

Variability in iodine value is observed in kernels according to their dry matter content. However, this variability does not exist in whole or crushed seeds with different dry matter contents.

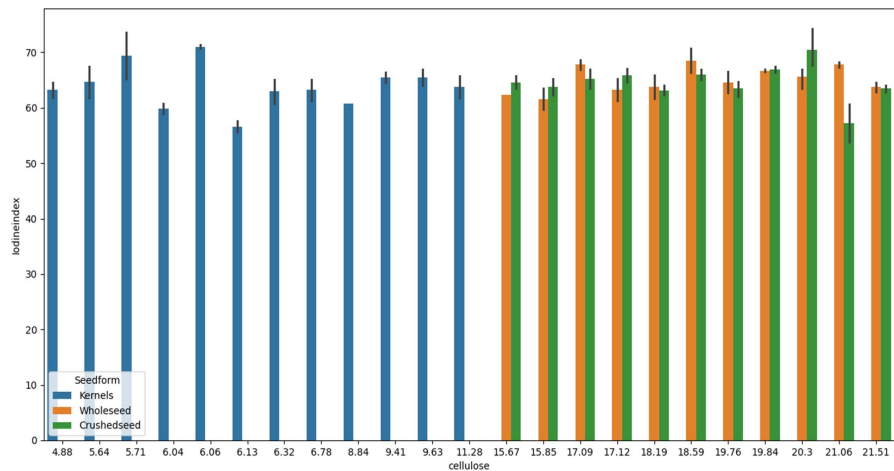


Figure 9. Iodine index as a function of cellulose content of jatropha seed oil.

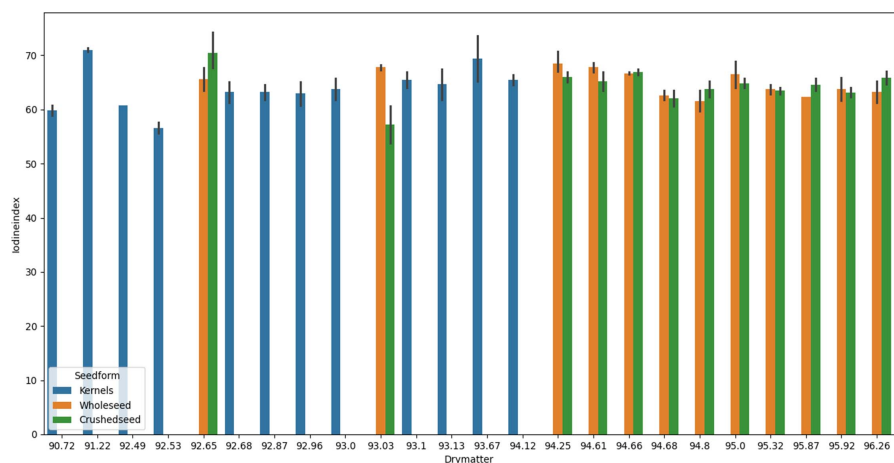


Figure 10. Iodine index as a function of dry matter content of jatropha seed oil.

The highest iodine value was observed in kernels with a dry matter content of 93.67%, and the lowest value was obtained in crushed seeds with a dry matter content of 93.03%.

3.5.4. Peroxide Index as Function of Cellulose Content

Figure 11 illustrates the peroxide value as a function of cellulose content: Whole seeds with a cellulose content of 15.67% had the highest peroxide value. In contrast, jatropha kernels had the lowest peroxide values and the lowest cellulose content. The lowest peroxide value, however, was observed in kernels with a cellulose content of 9.63%.

Regardless of the shape of the seeds or their cellulose content, the peroxide value ranges from 10 to 24 meq KOH/kg.

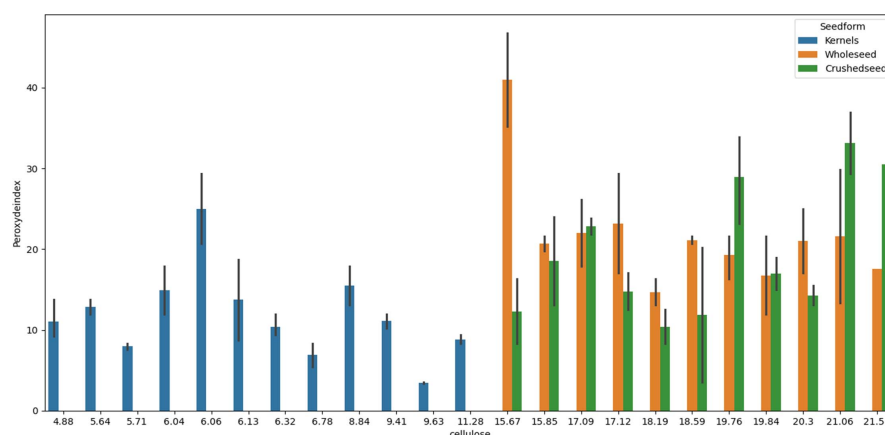


Figure 11. Peroxide index as a function of cellulose content.

3.5.5. Peroxide Index as Function of Lipid Content

Figure 12 illustrates the relationship between peroxide value and lipid content. Kernels with the highest lipid content had the lowest peroxide values. The lowest observed peroxide value for kernels was 38.87%.

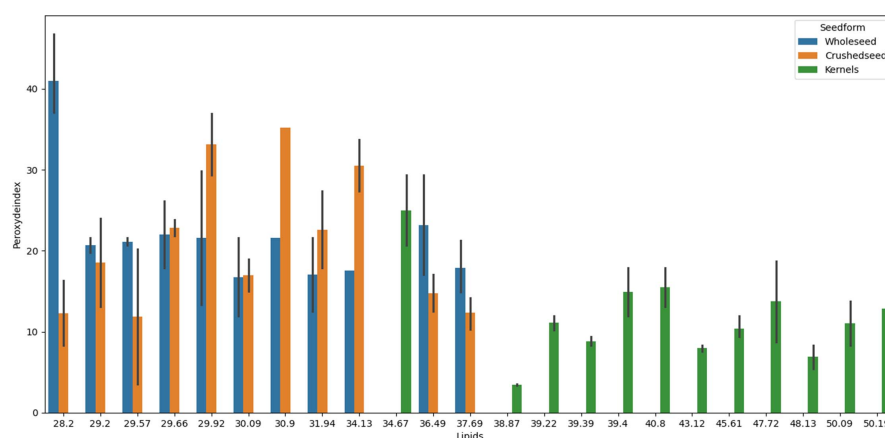


Figure 12. Peroxide index as function of lipid content of jatropha seed oil.

In contrast, whole and crushed grains achieved the highest peroxide values at lower lipid contents. The highest peroxide value was obtained at a lipid content of 28.2%.

3.5.6. Peroxide Index as Function of Dry Matter Content

Figure 13 illustrates the relationship between peroxide value and dry matter content. Kernels generally had the lowest peroxide values, with dry matter contents ranging from 90% to 94%.

Despite their high dry matter content, whole and crushed seeds achieved the highest peroxide values. Whole seeds with a dry matter content of 95.87% had the highest peroxide value.

3.5.7. Acid Index as Function of Dry Matter Content

Figure 14 illustrates the acidity index as a function of dry matter content. As be-

fore, almonds with lower dry matter content had the lowest acidity indices. However, kernels with a dry matter content of 92.87% had the lowest Acid index. Similarly, both whole and crushed seeds exhibit the highest acidity levels. The primary finding is that crushed seeds exhibit the highest acidity index values at a dry matter content of 96.26%.

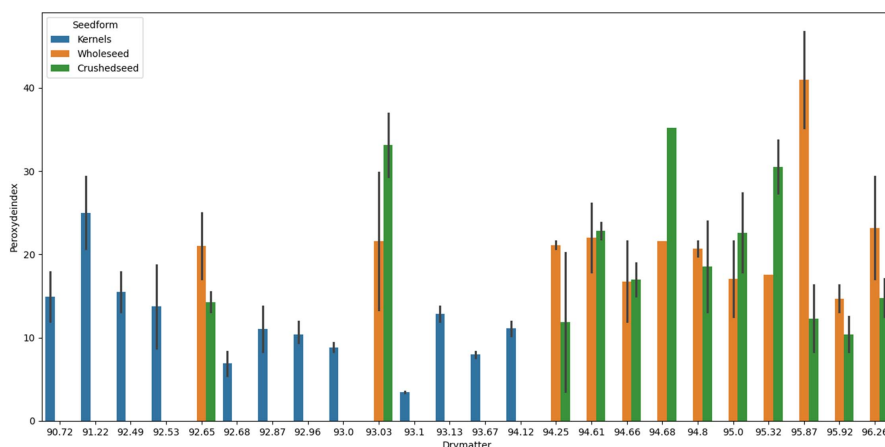


Figure 13. Peroxide index as a function of dry matter content.

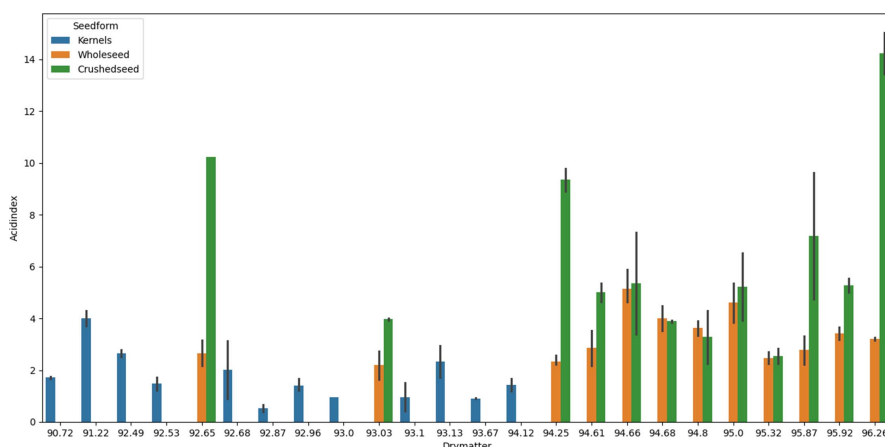


Figure 14. Acid index as function of drymatter content of jatropha seed oil.

3.5.8. Acid Index as Function of Cellulose Content

Figure 15 illustrates the relationship between acidity index and cellulose content. Kernels with low cellulose content produced the lowest acidity indices. However, kernels with a cellulose content of 4.88% had the lowest acidity index.

In general, crushed and whole seeds produced the most acidic results. Keep in mind that these seeds have a high cellulose content. However, crushed seeds with a cellulose content of 17.12% had the highest acidity index.

3.5.9. Acid Index as Function of Lipid Content

Figure 16 illustrates the acidity index of extracted oils as a function of seed lipid content. Generally, the highest acidity indexes were observed for whole and crushed seeds at lower lipid contents. The lowest acidity index was obtained for

crushed seeds with a lipid content of 36.49%.

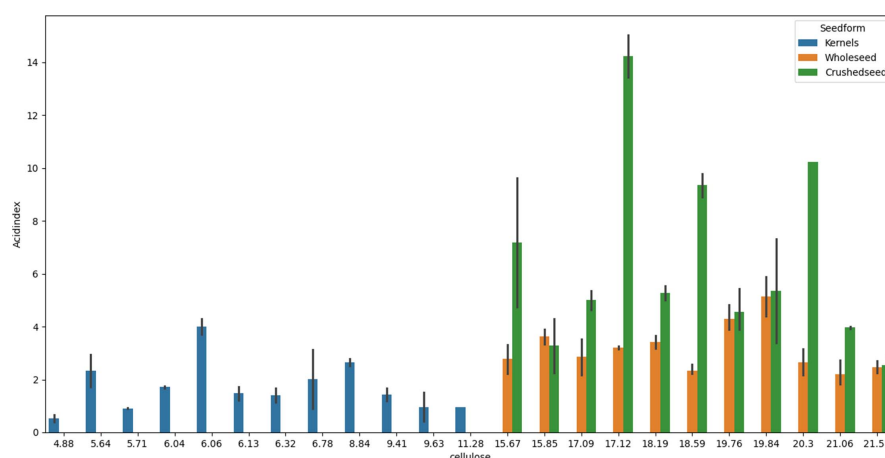


Figure 15. Acid index as function of cellulose content of jatropha seed.

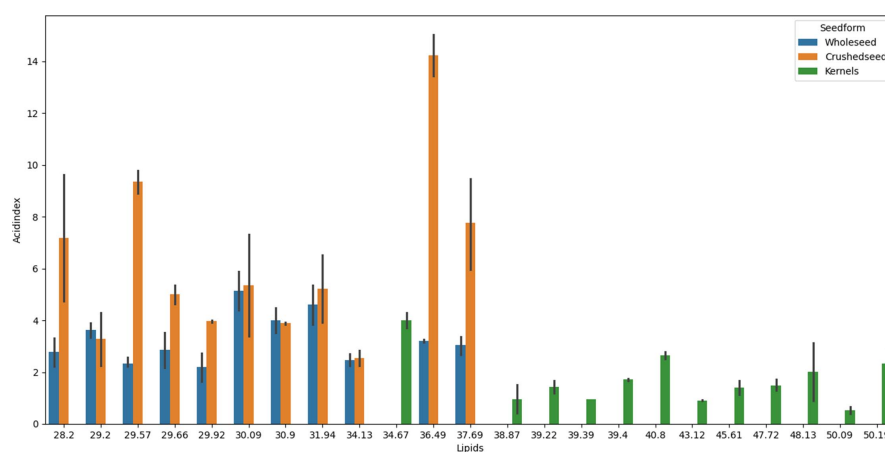


Figure 16. Acid index as function of lipid content of jatropha seed.

As shown on the graph, oils derived from high-fat kernels had the lowest acid content. The lowest acidity index was obtained from kernels with 38.87% lipids.

3.6. Optimization Process Using Response Surface Methodology

3.6.1. Quadratic Model of the Peroxide Index (meq KOH/kg Oil)

The optimization process of peroxide, iodine, and acid values was established based on the lipid, cellulose, and dry matter contents corresponding to each set of *Jatropha* seeds (whole, kernel, and crushed). The coefficients of the polynomial equation related to the Box-Behnken design for each oil samples based on *Jatropha* seed types are presented in **Tables 6-8**, which correspond to the peroxide, iodine, and acid values, respectively.

Whole seeds appear to predict the peroxide value (meq KOH/kg) the best, followed by crushed seeds and kernels. The respective correlation coefficients are 0.71, 0.62, and 0.57. The Equations (4), (5) and (6) are presented below.

Table 6. Coefficient of the quadratic model corresponding to the peroxide index (meq KOH/kg).

Coefficients	Jatropha seed groups		
	Whole seed	Kernel	Crushed seed
β_1	2.015	1.127	1.965
β_2	5.26	4.130	1.448
β_3	1.600	2.130	0.413
β_4	0.140	1.847	-0.332
β_5	-1.755	4.762	-0.372
β_6	2.155	0.327	-2.4
β_7	-8.871	8.759	15.662
β_8	-5.806	-0.880	-3.820
β_9	-6.326	-2.610	7.314
R^2	0.715	0.571	0.629
RMSE	4.4	4.12	6.1

peroxide value for whole seed

$$\begin{aligned}
 &= (2.015 \times L) + (4.130 \times C) - (2.13 \times DM) + (1.847 \times L \times C) \\
 &\quad - (1.755 \times L \times DM) + (2.155 \times C \times DM) - (8.871 \times L^2) \\
 &\quad - (5.806 \times C^2) - (6.326 \times DM^2)
 \end{aligned} \quad (4)$$

peroxide value kernel seed

$$\begin{aligned}
 &= (1.127 \times L) + (4.130 \times C) - (2.13 \times DM) + (1.847 \times L \times C) \\
 &\quad + (4.762 \times L \times DM) + (0.327 \times C \times DM) - (8.759 \times L^2) \\
 &\quad - (0.88 \times C^2) - (2.610 \times DM^2)
 \end{aligned} \quad (5)$$

peroxide value for crushed seed

$$\begin{aligned}
 &= (1.965 \times L) + (1.448 \times C) - (0.413 \times DM) - (0.372 \times L \times C) \\
 &\quad - (0.372 \times L \times DM) - (2.4 \times C \times DM) + (15.662 \times L^2) \\
 &\quad - (3.820 \times C^2) + (7.314 \times DM^2)
 \end{aligned} \quad (6)$$

3.6.2. Quadratic Model of the Iodine Index (mg I₂/g Oil)

Table 7 shows the coefficients of the quadratic model applied to the iodine index based on the set of Jatropha seeds.

Table 7. Coefficient of the quadratic model corresponding to the iodine index (mg I₂/g oil).

Coefficients	Jatropha seed groups		
	Whole seed	Kernel	Crushed seed
β_1	-0.896	1.577	-2.232
β_2	-2.202	-1.083	0.335

Continued

β_3	-0.788	-0.751	-1.77
β_4	1.465	2.232	-0.082
β_5	-1342	3.097	-0.992
β_6	-0.885	-1.25	1.412
β_7	-0.004	-2.992	-4.507
β_8	-0.267	-0.57	-0.857
β_9	1.445	0.742	0.627
R^2	0.48	0.742	0.627
RMSE	2.15	2.33	2.3

The results show that kernels are the best predictor of the iodine index (mg I₂/g oil), followed by crushed and whole seeds. The respective correlation coefficients are 0.74, 0.62, and 0.48. The Equations (7), (8) and (9) are presented below

Iodine value for whole seed

$$= -(0.896 \times L) - (2.202 \times C) - (0.788 \times DM) - (1.342 \times L \times C) - (0.885 \times L \times DM) - (0.004 \times C \times DM) - (0.267 \times L^2) + (1.445 \times C^2) + (2.15 \times DM^2) \quad (7)$$

Iodine value for kernel seed

$$= (1.577 \times L) - (1.083 \times C) - (0.751 \times DM) + (2.232 \times L \times C) + (3.097 \times L \times DM) - (1.25 \times C \times DM) - (2.992 \times L^2) - (0.57 \times C^2) + (4.785 \times DM^2) \quad (8)$$

Iodine value for crushed seed

$$= -(2.232 \times L) + (0.335 \times C) - (1.77 \times DM) - (0.082 \times L \times C) - (0.992 \times L \times DM) + (1.412 \times C \times DM) - (4.507 \times L^2) - (0.857 \times C^2) - (3.472 \times DM^2) \quad (9)$$

3.6.3. Quadratic Model of the Acidity Index

Table 8 shows the coefficients of the quadratic model applied to the acidity index (%) according to the *Jatropha* seed group. The correlation coefficients are 0.77, 0.72, and 0.35, respectively, showing that kernel *Jatropha* seeds are the best predictor of the acidity index, followed by crushed and whole seeds.

Table 8. Coefficient of the quadratic model corresponding to the acidity index (%).

Coefficients	Jatropha seed groups		
	Whole seed	Kernel	Crushed seed
β_1	-0.085	0.355	-0.64
β_2	-0.603	-0.08	-0.523

Continued

β_3	-0.451	-0.512	-673
β_4	0.13	0.585	-0.175
β_5	-0.495	0.405	1.18
β_6	-0.962	0.145	-0.122
β_7	0.032	0.493	1.099
β_8	1.835	0.718	0.462
β_9	0.215	0.473	0.517
R^2	0.355	0.774	0.72
$RMSE$	0.88	0.529	2.03

The corresponding models for each group of jatropha seeds are presented by Equations (10), (11) and (12).

$$\begin{aligned}
 &\text{Acid value for whole seed} \\
 &= -(0.085 \times L) - (0.603 \times C) - (0.451 \times DM) + (0.13 \times L \times C) \\
 &\quad - (0.495 \times L \times DM) - (0.962 \times C \times DM) + (0.032 \times L^2) \\
 &\quad + (1.835 \times C^2) + (0.215 \times DM^2)
 \end{aligned} \tag{10}$$

$$\begin{aligned}
 &\text{Acid value for kernel seed} \\
 &= (0.355 \times L) - (0.08 \times C) - (0.512 \times DM) + (0.585 \times L \times C) \\
 &\quad + (0.405 \times L \times DM) + (0.145 \times C \times DM) + (0.493 \times L^2) \\
 &\quad + (0.718 \times C^2) + (0.473 \times DM^2)
 \end{aligned} \tag{11}$$

$$\begin{aligned}
 &\text{Acid value for crushed seed} \\
 &= -(0.64 \times L) - (0.523 \times C) - (0.673 \times DM) - (0.175 \times L \times C) \\
 &\quad + (1.18 \times L \times DM) - (0.122 \times C \times DM) + (1.099 \times L^2) \\
 &\quad + (0.462 \times C^2) + (0.517 \times DM^2)
 \end{aligned} \tag{12}$$

3.6.4. Determination of Optimal Solutions for Quadratic Models

Table 9 shows the optimal values for lipid, cellulose, and dry matter content corresponding to peroxide, iodine, and acidity values. Regarding the peroxide value model, the optimal lipid content is higher for whole seeds, whereas kernels and crushed seeds have the same lipid content. Using the same model, the cellulose content is higher in crushed seeds than in whole seeds and kernels. Similar observations were made for dry matter content, though the lowest value was found in crushed seeds.

The iodine value model revealed that the lipid content of whole and crushed seeds was equivalent. However, the optimal cellulose content was the same for both. A similar observation was made regarding dry matter content. Crushed seeds exhibited the highest value. Finally, the acidity models revealed an identical lipid content value for whole and crushed seeds. The optimal cellulose content value was the same for kernels and crushed seeds, with the highest value recorded

for whole seeds. The three groups of seeds were found to have equivalent optimum dry matter content values. Considering these findings, the optimum values are significant for agronomy because they establish conditions for producing seeds with these lipid, cellulose, and dry matter characteristics.

Table 9. Optimal values for lipid, cellulose and dry matter contents of each jatropha seed sample.

Jatropha seed groups	Optimal values of parameter corresponding to peroxide value			Corresponding equations
	Lipid content (%)	Cellulose content (%)	Dry matter (%)	
Whole seed	37.69	15.67	96.26	4
Kernels	28.2	15.67	96.26	5
Crushed seeds	28.2	21.51	92.65	6
Optimal values of parameter corresponding to Iodine				
Whole seed	37.69	21.51	92.65	7
Kernels	28.2	21.51	92.65	8
Crushed seeds	37.69	15.67	96.26	9
Optimal values of parameter corresponding to acid value				
Whole seeds	37.69	21.51	92.65	10
Kernels	28.2	15.67	92.65	11
Crushed seeds	37.69	15.67	92.65	12

3.7. Decision Tree Results

3.7.1. Peroxide Value

Figure 17 and **Figure 18** illustrate the decision tree models used to predict the peroxide index based on the lipid, cellulose, and dry matter content of each jatropha seed sample. **Figure 18** indicates the model's robustness with a precision accuracy of 91%.

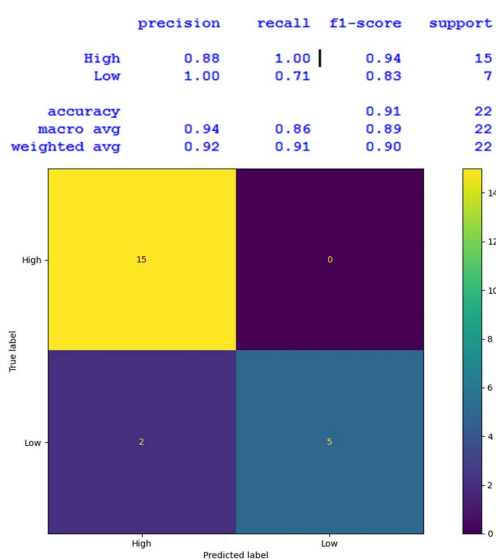


Figure 17. Peroxide value prediction using scikit learn.

It appears that the model classifies the peroxide index according to the quality of the bio-oil, distinguishing between high-quality and low-quality oils. As demonstrated in the existing literature [25]-[27], a peroxide value below 10 - 15 meq OH/kg oil indicates freshness and stability against oxidation. Conversely, a value above 30 meq OH/kg oil indicates rancidity and instability. An analysis of the training dataset revealed that the model accurately identified 20 bio-oil samples from each group of *Jatropha* seeds as high quality and misclassified only two samples. The model also provides reliable predictions. **Figure 18** shows the decision tree regression model. The correlation coefficient R^2 between the predicted and actual peroxide values is 0.54, corresponding to a residual error.

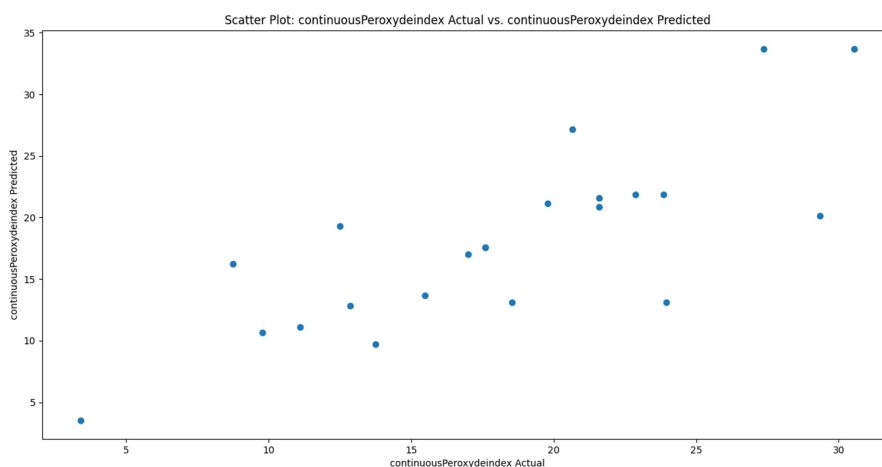


Figure 18. Peroxide value prediction.

Indeed, R^2 is considered satisfactory. This model can be used to predict the peroxide value based on the content of lipids, cellulose, and dry matter in the seed oil.

3.7.2. Iodine Value Prediction

Figure 19 and **Figure 20** demonstrate the decision tree model for predicting the iodine index as a function of the lipid, cellulose, and dry matter content of each group of *Jatropha* seeds. **Figure 19** shows that the precision-accuracy ratio is 95%, suggesting that the model is highly robust.

As shown in **Figure 19**, the model uses a classification system based on the iodine value of bio-oil to distinguish between high- and low-quality samples. Bio-oil derived from *Jatropha* oil is considered high-value when its iodine value is below 1.20 g I₂/g [30] because it has lower levels of unsaturation and greater stability against oxidation. In the present study, three levels of bio-oil were identified based on iodine value. These levels were designated as low, high, and very high. According to the previous analysis, all 19 bio-oil samples derived from each group of *Jatropha* seeds in the training dataset were correctly identified as having high bio-oil characteristics (lower iodine index value). Conversely, the model misclassified one sample.

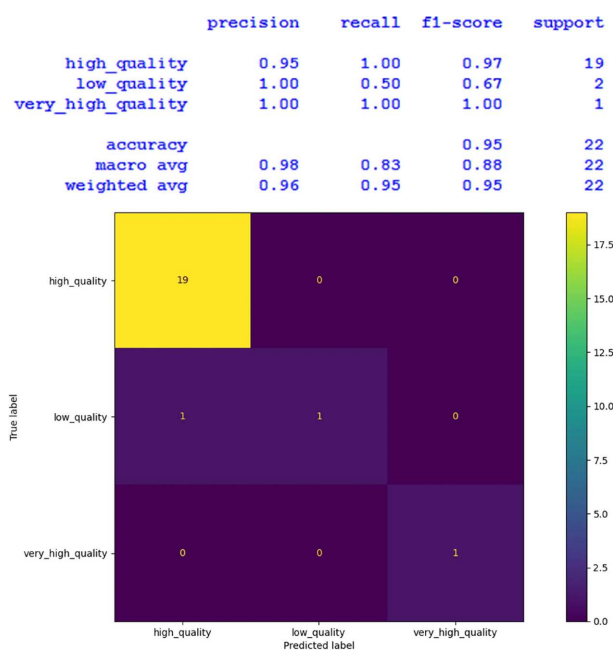


Figure 19. Iodine value prediction using scikit learn.

As illustrated in **Figure 20**, a decision tree regression model was employed. Clearly, the coefficient of determination, R^2 , between the predicted and actual iodine values is 0.5, corresponding to a mean square error of 5.72.

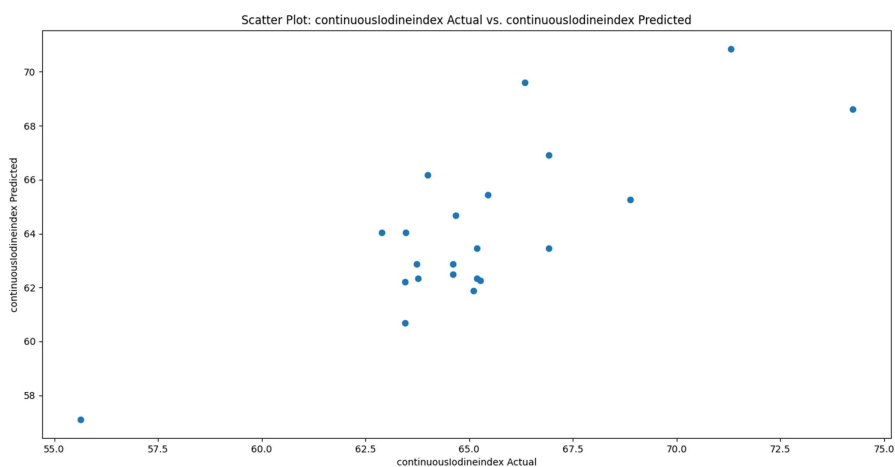


Figure 20. Iodine index prediction.

Indeed, R^2 is relatively acceptable. As the scatter plot shows, the model is a viable tool for predicting the Iodine value based on the lipid, cellulose, and dry matter content of the seed oil in question.

3.7.3. Acid Value

Figure 21 and **Figure 22** illustrate the decision tree model used to predict the iodine index based on the lipid, cellulose, and dry matter content of each *Jatropha* seed group. **Figure 21** shows that the model is highly robust, with a precision-

accuracy of 95%.

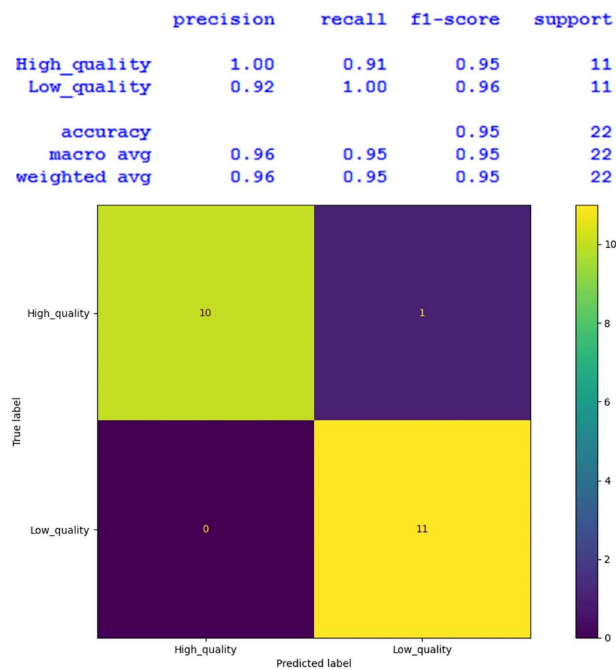


Figure 21. Acid value prediction using scikit learn.

Figure 21 shows that the model uses a classification system based on acid value to differentiate between high- and low-quality bio-oil. Bio-oil derived from *Jatropha* seeds exhibits acid values below 2% and above 5%, respectively [17] [30]. In this study, the model accurately identified 21 samples of bio-oil from each group of *Jatropha* seeds as having high or low levels of bio-oil characteristics (*i.e.*, higher or lower acid index values) within the training dataset, as previously outlined. The model misclassified only one sample.

Figure 22 shows the regression model of the decision tree. The R^2 coefficient of determination between the predicted and actual acid values appears to be 0.9, corresponding to a mean square error of 0.44.

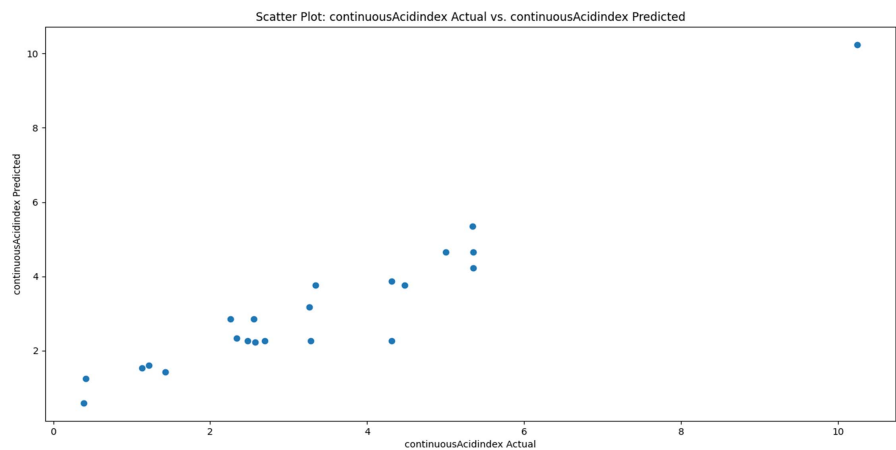


Figure 22. Acid value prediction.

In fact, R^2 is relatively acceptable. According to the scatter plot, the model can predict the peroxide value based on the lipid, cellulose, and dry matter content of the seed oil.

4. Conclusion

This study aimed to evaluate and predict the bio-oil characteristics (acid value, peroxide index, and iodine value) of Cameroonian *Jatropha curcas* treated as whole, kernels, and crushed seeds using machine learning techniques (response surface methodology and decision trees). Multiple regression models and a decision tree were employed based on the measured data collected from the seed oil extraction of the above three *Jatropha* seed samples. There was no significant difference among *Jatropha* seeds sample in terms of iodine index values. However, the three *jatropha* seed samples showed significant differences in acidity and peroxide indices. Additionally, the physicochemical properties of the bio-oils fall within ranges that comply with international standards. Predicting bio-oil characteristics based on three seed samples using machine learning is satisfactory. The correlation coefficients between the physicochemical properties of bio-oils (peroxide indices, iodine, and acidity) and the physicochemical properties of *jatropha* seeds (lipid, cellulose, and dry matter content) are in the range of 0.5. Decision tree predicting the chemical properties of bio-oils as a function of *jatropha* seed sample. In fact, model's robustness shows a precision accuracy of 91%, 95% and 95% for peroxide index, acid value and iodine index respectively. In addition, the coefficient of correlation was satisfactory corresponding to 0.54, 0.5 and 0.9 for peroxide index, iodine index and acid value respectively. Finally, response surface methodology using Box-Behnken design determined the optimal values for lipid content, cellulose, and dry matter, which would be valuable for optimizing *jatropha curcas* cultivation techniques for industrial biofuel production in Cameroon. Future research will study the impacts of other variation factors like the storage conditions, seed maturity and the growth area on the physicochemical properties of bio-oil for further improvement and application of Machine learning to develop the bio-fuel industry in Cameroon.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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