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*Research Article*

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**Special Issue**
*A Themed Issue in Honour of Professor Onukwuli Okechukwu Dominic (FAS).*

This special issue is dedicated to Professor Onukwuli Okechukwu Dominic (FAS), marking his retirement and celebrating a remarkable career. His legacy of exemplary scholarship, mentorship, and commitment to advancing knowledge is commemorated in this collection of works.

Edited by
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# Soft computing optimization of vegetable oil extraction

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**Abstract**
The introduction of machine learning in prediction of yield for bioprocessing is stimulating the wide usage of the first-generation biomass (vegetable oil) especially in production of biodiesel and biolubricant. This study focused on soft computing optimization of gmelina seed oil extraction using ANN and ANFIS. The results showed that ANN is better tool for prediction of oil yield with highest coefficient of determination of 0.998 and minimum error of 0.241. The optimal GSO yield of 50.4% was obtained when these factors were adjusted to 1.5mL/mg, 45minutes, 50ºC, 0.55mm, and 200rpm. This provides a crucial step towards developing a sustainable and renewable energy source, which has the potential to positively impact both the environment and local communities.
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**Keywords:** Artificial neural networks, adaptive neuro fuzzy inference systems, gmelina seed oil, extraction, optimization.

## 1. Introduction

The worldwide demand for oil seeds is projected to rise significantly in the next three decades, driven by increasing consumption of edible oil, the expansion of the biofuel sector, and the push for sustainable chemical processes. Currently, global oil production is approximately 135 million tonnes per year, with palm, soybean, and rapeseed oils contributing 30.9%, 23.9%, and 15.1% of total output, respectively (Avram et al., 2014; Kaniapan et al., 2021). Vegetable oils play a vital role in various industries, including food, energy (biofuels), and chemicals, with current attention shifting towards biofuels, especially biodiesel, which can be derived from non-edible seed oils (Zabermawi et al., 2022).

Numerous edible and non-edible oils are under investigation for biodiesel production, with growing interest in non-edible varieties. Research is focusing on various non-edible vegetable oil sources as alternatives to conventional options, including tallow seed (Maduelosi et al., 2019), castor (Dejene et al., 2022), sunflower (Alaei et al., 2018), canola (Kim et al., 2018), rubber seed (Herawati et al., 2022), jatropha curcas (Hussain et al., 2023), neem (Dash et al., 2021), cottonseed (Ude et al., 2020), Dacryodes edulis seed oil (Onukwuli & Ude, 2018), and gmelina seed oil. Notably, the potential of gmelina oil as a sustainable biodiesel source remains largely untapped.

Gmelina arborea Roxb is a large forest tree valued for its wood, which is used in furniture making and construction. This fast-growing tree flourishes in various locales, particularly in moist, fertile valleys with rainfall ranging from 750 to 5000 mm. Only a few studies have investigated the production of biodiesel from gmelina seed oil, such as Ude and Onukwuli (2019), who examined the kinetic study of the alcoholysis of gmelina seed oil using an base modified clay catalyst. Research on Gmelina seed oil is critical for its potential to contribute significantly to the development of a sustainable biodiesel industry. The oil extracted from its seeds has a unique fatty acid profile, containing predominantly oleic acid, making it an attractive candidate for biodiesel production. Moreover, Gmelina seed oil has a high iodine value, which allows for improved cold flow properties and cetane number, reducing the freezing points and improving the engine performance in colder climates. Ultimately, Gmelina seed oil offers a promising, eco-friendly, and economically viable alternative to conventional diesel fuels (Ude & Onukwuli, 2019). This can be achieved by optimizing the oil extraction from the seed. The broader application of most non-edible oils is constrained by inadequate modeling of their extraction processes using soft computing methods.

In search of optimal bioprocessing conditions, researchers are exploring modeling, predicting, and optimizing process parameters utilizing Responses Surfaces Methodology (RSM), Artificial Neural Networks (ANN), and Adaptive Neuro-Fuzzy Inferences Systems (ANFIS) (Dadhania et al., 2021; Ingie et al., 2023; Nwosu-Obieogu et al., 2024). RSM evaluates linear, interaction, and quadratic effects to identify ideal operating conditions for processes (Marzouk et al., 2021; Samuel et al., 2020; Ude et al., 2020; Fakhari, 2023). While RSM has been used for oil extraction from seeds, it has limitations, such as the inadequacy of models for extrapolation beyond experimental ranges and its struggles with complex variables. In contrast, soft computing methods like ANN and ANFIS have demonstrated superior predictive capabilities (Okeleye and Betiku, 2019; Samuel et al., 2022; Belmajdoub and Abderaft, 2023). ANN is a powerful tool for pattern recognition and regression analysis, capable of learning from vast datasets to identify underlying trends. However, it can sometimes act as a "black box," lacking transparency in how it derives outputs. On the other hand, ANFIS combines the learning capabilities of neural networks with the human-like reasoning of fuzzy logic, allowing for greater interpretability and flexibility (Ude et al., 2020; Nwosu-Obieogu et al., 2024). By employing both models, researchers can leverage ANN's efficiency in processing data while benefiting from ANFIS's ability to enhance interpretability and adaptability, leading to more robust and insightful conclusions in complex problem domains. Information on seed oil extraction through ANN and ANFIS remains limited. Therefore, this study aims to utilize soft computing techniques to model the extraction of oil from gmelina seeds.

## 2.0 Materials and methods

### 2.1 Materials

The seeds were gathered from premises of Energy Research Centre at the University of Nigeria, Nsukka, Enugu State, Nigeria. They were sun-dried, shelled, and then ground with a grinder to aid in oil extraction. N-hexane was utilized for the oil extraction process. All chemicals and solvents utilized were of analytical grade and obtained from commercial suppliers without any additional processing.

### 2.2 Methods

#### 2.2.1 Oil extraction

The technique described by Onukwuli and Ude (2018) were utilized to extract the oil. The extraction of the oil was evaluated through solvent extraction, using 100 grams of crushed kernels. The kernels were ground and combined with n-hexane (boiling point 40-60°C) at a solvent-to-kernel ratio varying between 0.5 ml/g and 2.5 ml/g. This mixture was agitated with a magnetic stirrer at a steady speed of 200 rpm, maintained within a temperature range of 30°C to 70°C for a duration of 15 to 75 minutes. The ranges of the parameters were selected based on previous study on extraction of oil by Uzoh and Onukwuli (2014). Following the extraction, the mixture was filtered using a vacuum filtering system that included a Millipore glass base and funnel. The amount of residual oil in the flask was measured after the end of the process.

The crude oil's yield was determined by applying Equation (1).

$$\text{GSOY} = \frac{W_o}{W} * 100 \quad (1)$$

Where, GSOY is gmelina seed oil yield (%),
$W_o$ is the quantity of the extracted oil (g) and
W is the quantity of the seed (g).

### 2.2.2 Soft Computing of the Oil Extraction

The extraction of oil from gmelina seed was modelled with artificial neural network (ANN) and adaptive neuro-fuzzy inference systems (ANFIS) using design matrix generated by Design Expert version 13. The dependent variable is oil yield while the independent variables are fraction of temp., solvent/solutes ratio, duration, particle sizes, and speed with a total of 32 experimental runs (Table 1).

**Table 1: Response of Experimental Design Matrix**

| Solvent/solid ratio (ml/mg) | Time (Minutes) | Temperature (°C) | Particle size ($\mu m$) | Agitation Speed (rpm) | Oil Yield (%) | ANN Predicted Yield (%) | ANFIS Predicted Yield (%) |
|---|---|---|---|---|---|---|---|
| 1 | 30 | 40 | 0.4 | 250 | 37 | 36.97 | 37.00 |
| 2 | 30 | 40 | 0.4 | 150 | 32.5 | 32.50 | 32.50 |
| 1 | 60 | 40 | 0.4 | 150 | 27.8 | 27.79 | 27.80 |
| 2 | 60 | 40 | 0.4 | 250 | 28.5 | 28.48 | 28.50 |
| 1 | 30 | 60 | 0.4 | 150 | 37 | 37.07 | 37.00 |
| 2 | 30 | 60 | 0.4 | 250 | 30 | 29.99 | 29.99 |
| 1 | 60 | 60 | 0.4 | 250 | 32 | 32.01 | 31.99 |
| 2 | 60 | 60 | 0.4 | 150 | 33.5 | 33.39 | 33.50 |
| 1 | 30 | 40 | 0.7 | 150 | 33 | 33.04 | 33.00 |
| 2 | 30 | 40 | 0.7 | 250 | 35 | 35.03 | 34.99 |
| 1 | 60 | 40 | 0.7 | 250 | 36 | 36.01 | 35.99 |
| 2 | 60 | 40 | 0.7 | 150 | 31.5 | 31.50 | 31.49 |
| 1 | 30 | 60 | 0.7 | 250 | 28 | 27.99 | 28.00 |
| 2 | 30 | 60 | 0.7 | 150 | 33 | 32.98 | 33.00 |
| 1 | 60 | 60 | 0.7 | 150 | 29 | 28.96 | 28.99 |
| 2 | 60 | 60 | 0.7 | 250 | 33 | 33.07 | 33.00 |
| 0.5 | 45 | 50 | 0.55 | 200 | 40 | 40.09 | 40.00 |
| 2.5 | 45 | 50 | 0.55 | 200 | 39 | 38.99 | 39.00 |
| 1.5 | 15 | 50 | 0.55 | 200 | 34.5 | 34.53 | 34.50 |
| 1.5 | 75 | 50 | 0.55 | 200 | 31 | 30.99 | 31.00 |
| 1.5 | 45 | 30 | 0.55 | 200 | 40 | 39.98 | 40.00 |
| 1.5 | 45 | 70 | 0.55 | 200 | 38 | 38.24 | 38.00 |
| 1.5 | 45 | 50 | 0.25 | 200 | 35.5 | 35.45 | 35.50 |
| 1.5 | 45 | 50 | 0.85 | 200 | 35 | 35.04 | 35.00 |
| 1.5 | 45 | 50 | 0.55 | 100 | 32 | 32.10 | 31.99 |
| 1.5 | 45 | 50 | 0.55 | 300 | 32.5 | 32.49 | 32.50 |
| 1.5 | 45 | 50 | 0.55 | 200 | 49 | 50.06 | 50.40 |
| 1.5 | 45 | 50 | 0.55 | 200 | 49 | 50.06 | 50.40 |
| 1.5 | 45 | 50 | 0.55 | 200 | 51 | 50.06 | 50.40 |
| 1.5 | 45 | 50 | 0.55 | 200 | 52 | 50.06 | 50.40 |
| 1.5 | 45 | 50 | 0.55 | 200 | 51 | 50.06 | 50.40 |

### 2.2.3 ANN modeling

The multi-variable-single output (MISO) neural architecture (Figure 1) was implemented to model the oil extraction process. The independent variables are listed in Table 1, while the single output represents the oil yield. The dataset in Table 1 was duplicated, and the number of neurons was adjusted to prevent overtraining and overfitting. Consequently, sixty-four (64) sets of data were utilized for training, and the data was analyzed using the logsig nonlinear transfer function in the hidden layer, along with the purelin function in the output layer. As noted by Ude et al. (2022), the network was trained with seventy percent of the data, representing 44 samples, while fifteen percent was allocated for both testing and validation, with each comprising 10 samples. The model's performances were assessed with mean square errors (MSE) and the coefficients of determination.

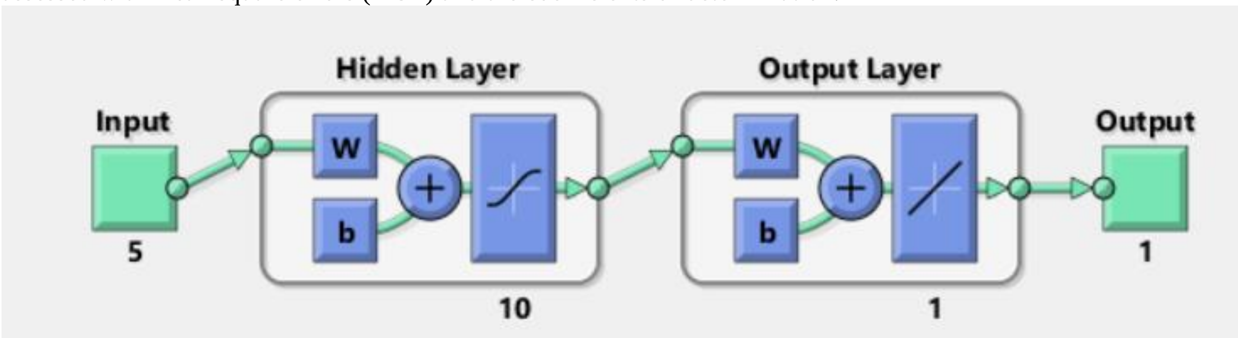



**Figure 1: MISO neural architecture.**

**2.2.4 ANFIS modelling**

The ANFIS network designs employed five distinct layers, including the fuzzy process, output, rule, defuzzy process, and total addition layers (Ude et al., 2022). For this study, the first-order Sugeno model was applied, using an input variable for oil yield (Figure 2). The fuzzy rules implemented were based on the IF-THEN rules developed by Takagi and Sugeno, as referenced by Betiku et al. (2018) and Ude et al. (2022). The modeling was conducted using the fuzzy logic toolbox in MATLAB R2013a.

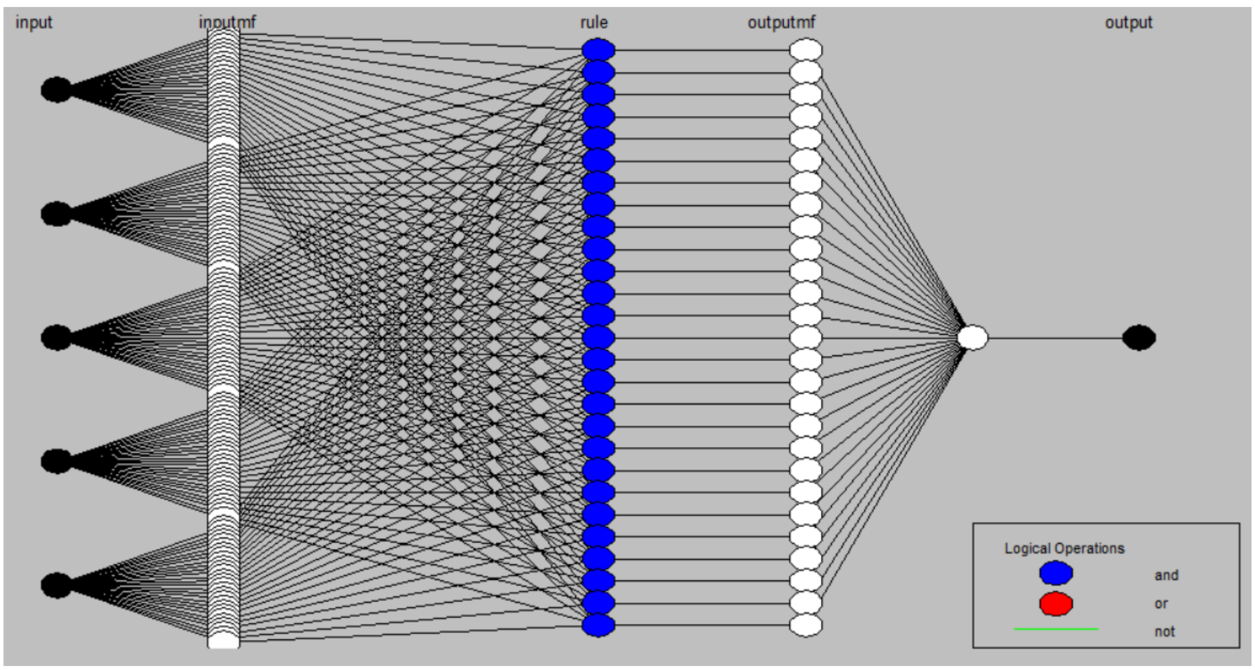



**Figure 2. ANFIS architecture for modelling Oil extraction.**

**2.2.5 Statistical Evaluation of the models**

The performance of each model was validated by assessing statistical metrics including root-mean-square error (RMSE), coefficients of determination ($R^2$), and coefficients of regression (R). The statistical indicators were evaluated using Equations. (2) – (4), as outlined by Ude et al. (2022).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(w_{a.i} - w_{p,i})^2} \quad (2)$$

$$R = \frac{\sum_{i=1}^{n}(w_{p,i} - w_{p,ave}).(w_{a,i} - w_{a,ave})}{\sqrt{[\sum_{i=1}^{n}(w_{p,i} - w_{p,ave})^2][\sum_{i=1}^{n}(w_{a,i} - w_{a,ave})^2}} \quad (3)$$

$$R^2 = \frac{\sum_{i=1}^{n}(w_{p,i} - w_{a,i})^2}{\sqrt{\sum_{i=1}^{n}(w_{a,ave} - w_{p,ave})^2}} \quad (4)$$

## 3.0 Result and Discussion

### 3.1 ANN Modelling of Gmelina Seed oil Extraction

The artificial neural network (ANN) was utilized to forecast the oil extraction parameters, employing a supervised learning approach. Figure 3 illustrates the network's training performance, revealing a mean square error of 0.24 for the prediction of oil yield at a maximum epoch of 5, indicating commendable performance with minimal errors. Additionally, Figure 4 presents the model's plot for oil yield prediction, demonstrating a strong correlation between the predicted and actual yields. The correlation coefficient exceeded 0.99, suggesting that the model effectively predicted the oil yield.

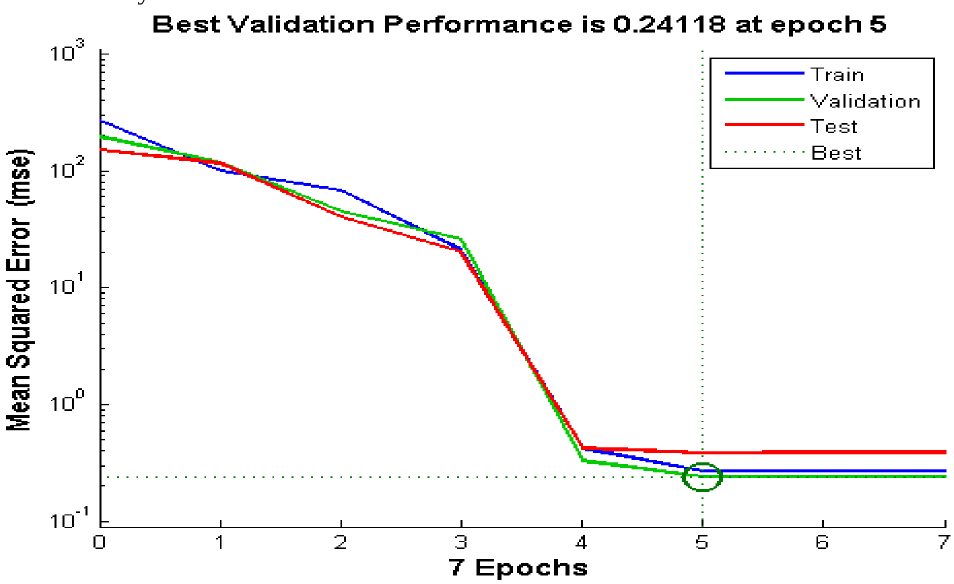



**Figure 3: MISO Performance Error for Predicting of Oil Yield.**

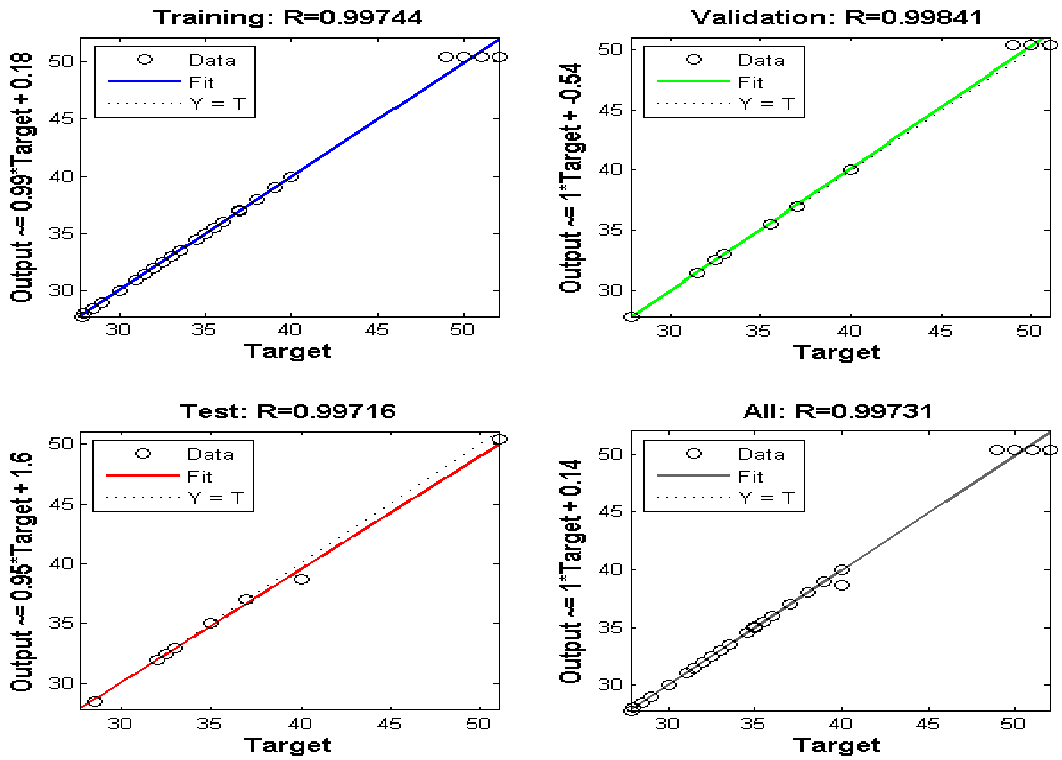



**Figure 4: MISO Regression Analysis for Oil Yield Prediction.**

### 3.2 ANFIS Modelling

The responses from the experimental design matrix for extracting oil from gmelina seeds were modeled using the ANFIS approach, as shown in Table 1. Figure 5 illustrates the correlation between the actual and generated yields for the ANFIS oil extraction model. The model achieved a $R^2$ of 0.9899, with an error of 0.48193, as demonstrated in Figure 5. The high $R^2$ value and the low average testing error indicate a strong correlation between the actual and generated results, with the model accounting for 98.99% of the variability observed.

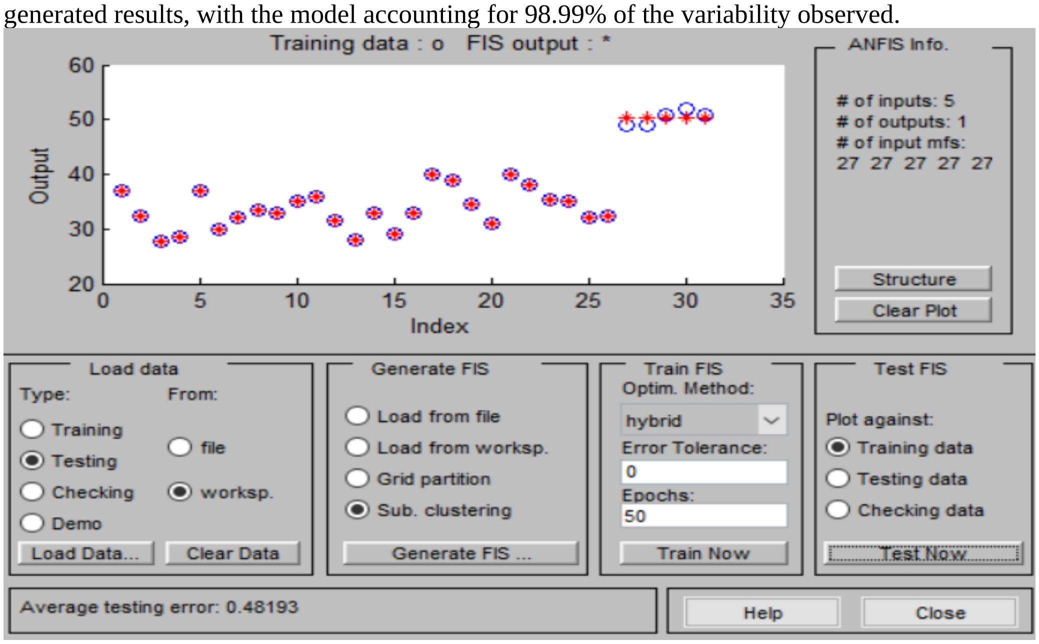


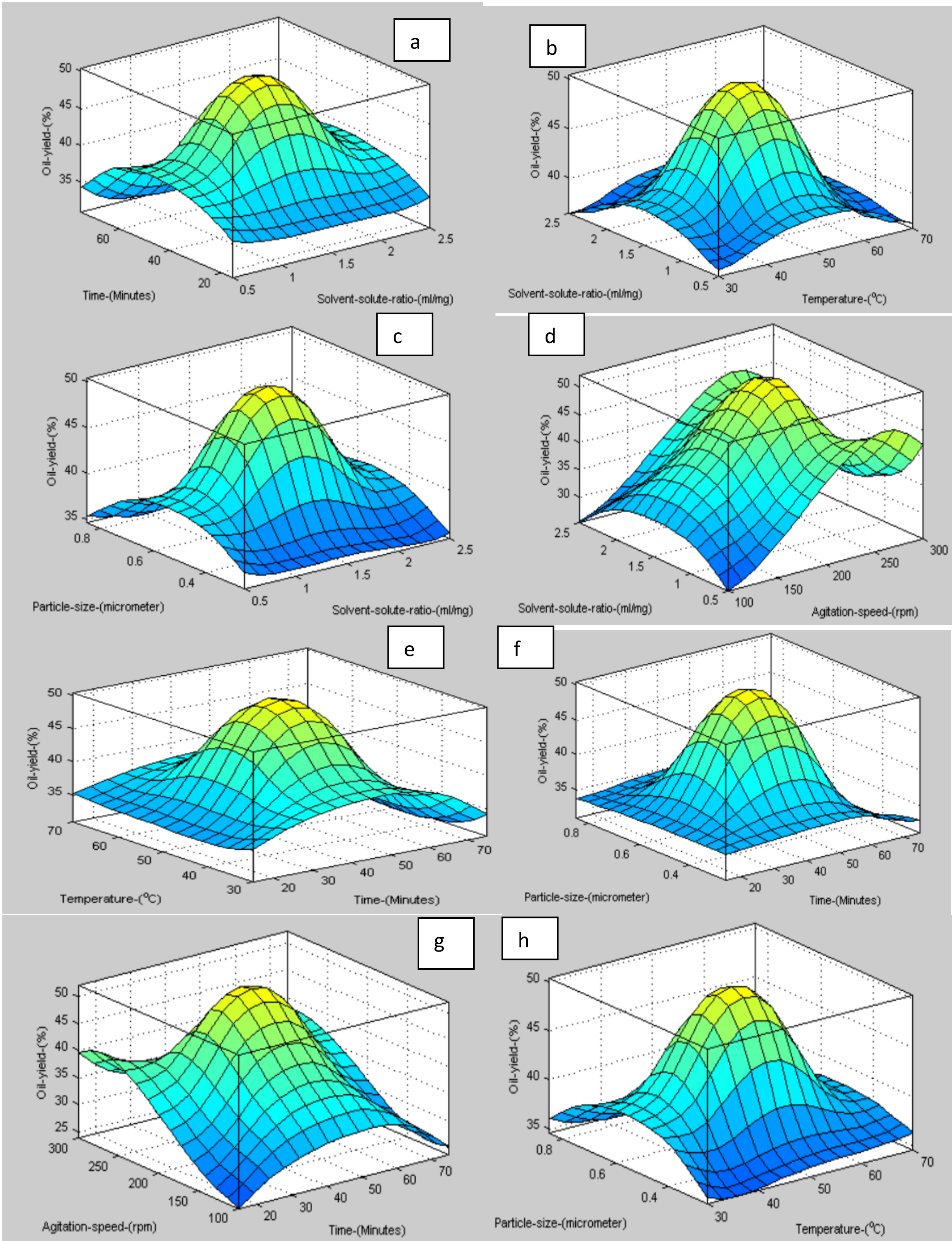

**Figure 5: Experimental and predicted oil yield**

Additionally, surface plots were created to assess the impact of various combinations of extraction factors on oil yield, and these are presented in Figure 6 (a-j). Specifically, Figure 6a illustrates the interactive influence of the solvent/solute ratio (SSR) and time on the yield of Gmelina seed oil extraction. It is evident that as both the SSR and time rose, the oil yield also increased, then started to decline after 1.6 mL/g and 60 minutes. This decrease in quantity of oil may be due to the evaporation of the solvent over extended exposure. Figure 6b illustrates how temperature and SSR interact to influence the yield of Gmelina seed oil. The figure indicates that while both increasing temperature and solvent/solute ratio enhance oil yield, yields decline when temperature exceeds 60°C and the ratio surpasses 1.6 ml/g. This decrease in yield at elevated temperatures could be linked to solvent evaporation once the temperature exceeds its boiling point.

In Figure 6c, the combination between solvent/solute ratio and particle size on GSO yield is depicted. It is evident from the plot that oil yield rises with rising SSR and a decreasing particle size. This improvement can be due to the greater surface area of the seeds that allows for more effective oil recovery at reduced particle sizes. Figure 6d illustrates the combined influence of SSR and speed on oil yield. The figure reveals that as both the SSR and speed rises, so does the oil yield, although there is a noticeable decline beyond 1.6 ml/g and 200 rpm. This reduction in yield may be due to the mass transfer limitations associated with increased agitation. The interaction between time and temperature on oil yield is shown in Figure 6e. It can be seen that oil yield rises with increased time and temperature, yet begins to decrease once these parameters surpass 60 minutes and 60°C, respectively. This decline in yield at higher temperatures may again be related to solvent evaporation occurring above its boiling point.

In Figure 6f, the interaction of time and particle size on oil yield is presented. The figure shows that as time increases and particle size decreases, oil yield improves, likely due to the larger surface area of the seeds at reduced sizes. Figure 6g demonstrates the interactive influence of time and speed on oil yield. The figure indicates that as both time and speed inclined, the oil yield also rises. This could be due to homogenized mixture provided by proper mixing which reduce mass transfer effect allowing the solvent to penetrate into the seed and enhanced oil yield. Similar results were reported by Ude and Onukwuli (2019) and Uzoh and Onukwuli (2014). Figure 6h illustrates how temp. and particle size interact to affect the yield of Gmelina seed oil (GSO). The data shows that oil yield rises with increasing temperature and decreasing particle sizes. This phenomenon can be demonstrated by the larger surface area of the seeds available for oil extraction when the particle size is smaller.

In Figure 6i, the relationship between temp. and speed on oil yield is depicted. The figure reveals that as both temp. and speed inclined, the oil yield also increases. However, there is a decline in yield when the temperature exceeds 60°C and agitation speed surpasses 200 rpm. This decline may be due to solvent evaporation occurring at elevated temperatures beyond its boiling point. Figure 6j presents the interaction between agitation speed and particle size on GSO yield. The plot indicates that quantity of oil improves as speed rises and particle size declines. This could be credited to the larger surface area of the seeds displayed for oil recovery when the particle size is reduced.


a
Oil-yield-(%)
Time-(Minutes)
Solvent-solute-ratio-(ml/mg)
b
Oil-yield-(%)
Solvent-solute-ratio-(ml/mg)
Temperature-(°C)
c
Oil-yield-(%)
Particle-size-(micrometer)
Solvent-solute-ratio-(ml/mg)
d
Oil-yield-(%)
Solvent-solute-ratio-(ml/mg)
Agitation-speed-(rpm)
e
Oil-yield-(%)
Temperature-(°C)
Time-(Minutes)
f
Oil-yield-(%)
Particle-size-(micrometer)
Time-(Minutes)
g
Oil-yield-(%)
Agitation-speed-(rpm)
Time-(Minutes)
h
Oil-yield-(%)
Particle-size-(micrometer)
Temperature-(°C)

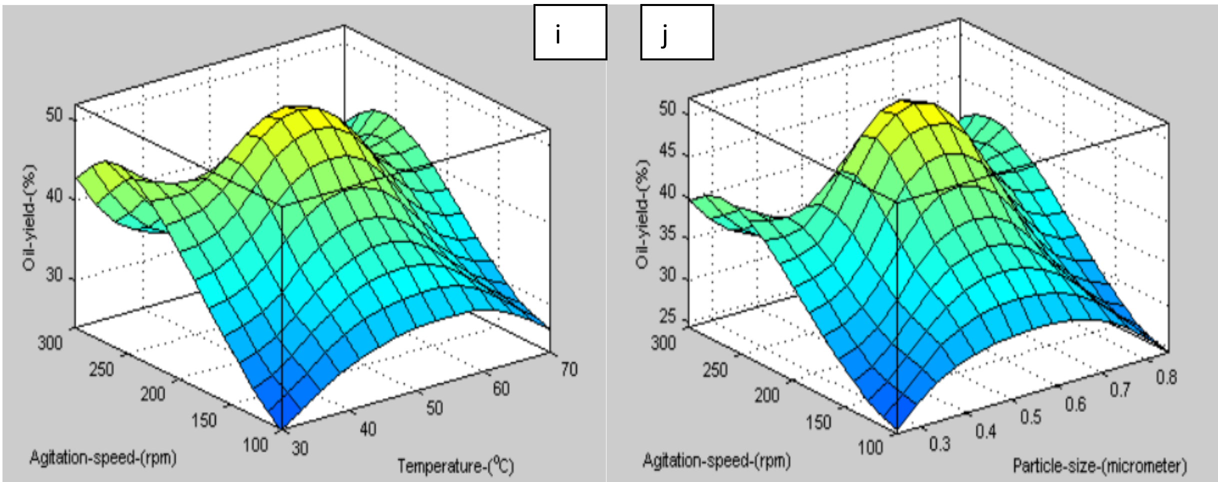



Figure 6: Surface Plots of the ANFIS model for interaction effect of: (a) solvent/solute ratio and time, (b) solvent/solute ratio and temp., (c) solvent/solute ratio and particle size, (d) solvent/solute ratio and speed, (e) time and temperature, (f) time and particle size, (g) time and speed, (h) temperature and particle size, (i) temp. and speed, (j) agitation speed and particle size.

The optimization of oil yield from gmelina seeds using n-hexane was conducted through ANFIS rules, focusing on the ideal SSR, extraction time, temp., particle size, and speed. The findings indicated that an oil yield of 50.4% from Gmelina seed oil (GSO) was achieved when these parameters were set to 1.5 mL/mg, 45 minutes, 50°C, 0.55 mm, and 200 rpm. Furthermore, the validation of the optimal extraction results showed a percentage error of less than 1%. The model demonstrated a strong capability to accurately predict outcomes, confirming its effectiveness in achieving optimal results.

### 3.3 Performance evaluation of the developed models

Statistical metrics were employed to assess the performance of the ANN and ANFIS models developed for predicting oil yield, with the results presented in Table 2. The $R^2$ and R values for the ANN model were slightly higher than those of the ANFIS model. Moreover, the ANN exhibited lower error rates compared to the ANFIS model, and both models displayed low calculated mean squared errors (MSEs). This suggests that while the ANN is more effective in predicting vegetable oil extraction yield at 99.8% than the ANFIS model at 98.9%, both models are viable options for estimating oil yield.

**Table 2: Statistical Indices of the Model**

| Index | ANN | ANFIS |
|---|---|---|
| $R^2$ | 0.998 | 0.989 |
| R | 0.999 | 0.994 |
| MSE | 0.24118 | 0.48193 |

### 3.4 Determination of the GSO Features

#### 3.3.1 Physical and chemical properties the GSO

Table 3 outlines the physical and chemical properties of the raw oil extracted from gmelina seeds. The oil exhibits a moderate level of acidity and a low free fatty acid content, suggesting that it is unlikely to need pre-treatment prior to transesterification with a homogeneous catalyst. However, its high density and viscosity could pose challenges for atomization in internal combustion engines, rendering it unsuitable for direct application as a biofuel. Conversely, the oil's low pour point exhibits that it will not solidify at absolute temperature, facilitating long-term storage. Additionally, the oil's high oxidation stability makes it a good candidate for biodiesel production, likely due to the solvent refining technique employed, which helps retain the natural antioxidants present in the base oil. In contrast, hydro-treated base oils typically necessitate extra antioxidant additives to ensure adequate thermal and oxidation stability.

**Table 3: Physic and chemical features of oil**

| S/N | Features | Gmelina pear seed oil |
|---|---|---|
| 1 | Sp. gra. | 0.90 |
| 2 | AV (mgKOHg) | 5.49 |
| 3 | FFA (%) | 2.71 |
| 4 | SV (mgKOH/g) | 41 |
| 5 | IV ($gI_2$/100g) | 34.9 |
| 6 | KV at 40$^oC$ ($mm^2/s$) | 7.9 |
| 7 | PV | 8.8 |
| 8 | FP | 214 |
| 9 | CP | -3 |
| 10 | PP | 16 |
| 11 | MC (%) | 7.1 |
| 12 | RI | 1.42 |
| 13 | Oxidation stability 11$^oC$ (Hour) | 6 |
| 14 | Molecular weight | 827.1 |

Sp. gra. = specific gravity, AV=acid value, FFA=free fatty acid, SV=saponification value, IV=iodine value, KV=kinematics viscosity, PV= peroxide value, FP=flash point, CP=cloud point, PP=pour point, MC=moisture content, RI=refractive index.

### 3.3.2 Fatty acid profile of the oil

The fatty acid profile of gmelina seed oil is detailed in Table 4. Gas Chromatography-Mass Spectrometry (GC-MS) analysis indicated high levels of oleic acid (41.86% weight), margaric acid (13.1% weight), palmitic acid (13.99% weight), and stearic acid (12.81% weight). Among the fatty acids, palmitic acid (14.20% weight) was identified as the predominant saturated fatty acid, while oleic acid (38.90% weight) was the most prevalent unsaturated fatty acid. Overall, the oil comprises 51.32% saturated fatty acids and 48.68% unsaturated fatty acids.

**Table 4: Fatty acid profile of Gmelina seed oil**

| S/N | FFA Profile | | Gmelina pear seed oil |
|---|---|---|---|
| | Fatty Acid | Component | Composition (%) |
| 1 | Capric acid | $C_{10}$ | 1.71 |
| 3 | Myristic acid | $C_{14}$ | 7.25 |
| 4 | Palmitic acid | $C_{16:0}$ | 13.99 |
| 5 | Magaric acid | $C_{17}$ | 13.1 |
| 6 | Stearic acid | $C_{18:0}$ | 12.80 |
| 7 | Oleic acid | $C_{18:1}$ | 41.86 |
| 9 | Linoleinic acid | $C_{18:3}$ | 6.82 |
| 10 | Arachidic acid | $C_{20}$ | 0.63 |
| 11 | Euric acid | $C_{21}$ | 1.84 |
| | Total | | 100 |

## 4.0. Conclusion

The research focused on optimizing the extraction of gmelina seed oil through soft computing techniques, specifically using Artificial Neural Networks (ANN) and Adaptive Neuro-Fuzzy Inference Systems (ANFIS). The findings indicated that ANN outperformed ANFIS in predicting oil yield, demonstrating the highest coefficient of determination and the lowest error rates. An optimal gmelina seed oil yield of 50.4% was achieved by adjusting the parameters to 1.5 mL/mg, 45 minutes, 50°C, 0.55 mm, and 200 rpm. This predictive model for oil extraction from seeds is expected to promote the broader use of non-edible oils for biodiesel and bio-lubricant production. Ultimately, this research represents a significant advancement in developing sustainable and renewable energy sources, which could have a beneficial effect on environmental health and local economies.

## 5.0 Recommendation

From the findings of the study, it is recommended that soft computing should be used to predict the yield of oil extraction and technoeconomic analysis of the extraction process should be studied.

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**Nomenclature**

ANFIS=Adaptive neuro-fuzzy inference systems;
ANN=Artificial neural method;
GSOY= Gmelina seed oil, %;
RMSE= Root mean square error;
MISO=Multi-input-single-output;
$W_o$ is the quantity of the extracted oil, g;
W is the quantity of the seed, g;

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