

Machine Learning Modeling and Global Optimization of Biodiesel Production from Waste-blend Feedstock using a Novel Copper-Doped Bio-derived Catalyst

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Abstract

High production costs, environmental concerns, and optimization complexities limit the viability of conventional biodiesel. To address this, a novel bio-based heterogeneous catalyst was prepared by impregnating Coconut Shell BioChar (CS-BC) with copper-doped calcined Periwinkle Shell (CPS). The morphology and stability of the catalyst were assessed using SEM, EDX, FTIR, XRD, and BET analyses. The catalyst was applied to transesterify an optimized blend of Waste Cooking Oil (WCO) and Animal Fat (AF). Modeling of the transesterification was conducted using Support Vector Regression (SVR), Artificial Neural Networks (ANN), Random Forest (RF), and Extreme Gradient Boosting (XGBoost), then globally optimized via the Manta Ray Foraging Optimization (MRFO). XGBoost outperformed the other models, achieving a coefficient of determination (R^2) of 0.899 with the lowest error metrics. SHAP analysis identified reaction temperature as the most influential feature. The MRFO established 66.3°C, 6.37 wt.% catalyst loading, 104.6 minutes, and an 8.84:1 methanol-to-oil ratio as the optimal conditions. Under these conditions, a maximum predicted biodiesel yield of 81.9% was achieved, closely matching the experimentally validated yield of $82.3 \pm 0.8\%$. The synthesized catalyst demonstrated high stability, retaining up to 97.1% of its activity after five consecutive reaction cycles. These findings highlight the catalyst's potential for sustainability and large-scale application. Physicochemical analysis confirmed that the produced biodiesel complies with ASTM D6751 and EN 14214 standards. This integrated framework of waste-derived feedstocks, green catalysis, and metaheuristic optimization offers a sustainable, data-driven approach to biofuel production.

Keywords: Biodiesel, Transesterification, Optimization, Machine learning modelling, Bifunctional Catalyst, Oil blend

1. Introduction

The energy transition worldwide necessitates the adoption of sustainable strategies to diversify the energy portfolio and minimize reliance on fossil fuels [1]. This has generated significant interest in alternative energy sources, leading to an increasing demand for sustainable energy alternatives. To serve as a viable substitute for fossil fuels, a renewable energy source must offer superior environmental sustainability, remain cost-effective, and scale sufficiently to make a meaningful impact on global energy demands. Biodiesel has become widely adopted globally due to its renewable nature, safety, biodegradability, high flash point, and lower environmental footprint relative to petroleum diesel [2]. As a green alternative to traditional diesel, biodiesel is produced from organic sources such as plant oils or animal fats. The standard approach relies on

transesterification using methanol [3, 4], a method widely preferred because it yields excellent results without requiring extreme conditions [5]. Extensive research on biodiesel production has primarily focused on reducing costs and optimizing resource utilization.

Feedstocks constitute the majority of biodiesel production costs, ranging from 70% to 95% [4, 6], with approximately 95% of the global supply currently derived from edible crops such as coconut, sunflower, palm, and soybean oils [7, 8]. This heavy dependence on food-grade resources has sparked a fierce "food-versus-fuel" debate, alongside critical challenges like deforestation and extensive occupation of arable land [9, 10]. Without careful planning, diverting edible agricultural crops to energy production threatens global food security and destabilizes economies

[11]. To address these rising costs, ethical concerns, and municipal waste challenges, the industry is shifting toward a sustainable circular economy by utilizing non-food alternatives such as jatropha, rapeseed, waste cooking oil, and waste animal fats [12]. While non-edible oils offer significant advantages, using them individually as feedstocks presents several challenges, including unstable and insufficient supply, inconsistent oil quality, and lower conversion efficiencies [13]. To overcome these limitations associated with relying on single inedible oil feedstocks for large-scale applications, researchers have proposed several solutions. One promising approach is blending two or more oil feedstocks in precise proportions. This method not only increases biodiesel yields but also improves the fuel properties of the resulting biodiesel through a positive synergistic effect [14]. This enhancement results from a synergistic interaction where the strengths of individual oils complement each other to deliver superior overall performance [15]. This oil blending strategy mitigates feedstock scarcity while improving fuel quality.

The economics of biodiesel production heavily depend on the nature and price of the catalysts used. Homogeneous catalysts such as sodium hydroxide and sulfuric acid are widely employed in commercial transesterification due to their fast reaction rates [20]. However, their use presents operational challenges, including catalyst loss during the reaction, equipment corrosion, and the need for extensive post-reaction washing. This washing process also produces large volumes of wastewater that may contain harmful substances [20, 23]. Consequently, the adoption of solid, cost-effective, and highly efficient catalysts offers significant potential as a breakthrough solution [17]. Solid catalysts have attracted considerable research interest because of key benefits such as reusability, high thermal stability, non-corrosive properties, and resistance to soap formation. Unlike liquid catalysts, which suffer from difficult separation, complex purification, and greater environmental risks, solid catalysts provide a more efficient and environmentally friendly alternative [18]. Another strategy to further reduce biodiesel production costs involves synthesizing solid catalysts from waste materials. These waste-derived precursors, abundantly available in African countries, especially Nigeria, contain the essential components necessary for producing heterogeneous catalysts [19]. Researchers are increasingly focusing on bio-based solid catalysts capable of handling both FFA esterification and triglyceride transesterification. This dual-

functionality approach reduces production costs while promoting sustainability within the biofuel sector [20, 21]. The dual acid-base activity is engineered by modifying carbon matrix supports with specific acidic and basic chemical precursors [22]. Prior studies demonstrate that various biomass wastes possess excellent potential as feedstocks for synthesizing bifunctional biodiesel catalysts. Successful examples include corn cobs combined with poultry droppings [23], rubber seed and eggshells [20, 21, 24], crab shells with plantain peels [25], and sugar industry waste [26]. Researchers have also effectively utilized cocoa pod husks [27], elephant ear pod husks [28], *Musa paradisiaca* (plantain) trunks, peels, and rhizomes [29], palm kernel shells [30], cow bones mixed with waste marble [31], periwinkle shells [32], coconut shells [33], and peanut shells [34].

Optimizing key reaction parameters is essential for achieving maximum biodiesel conversion [24]. Experimental models help quantify how specific variables influence product yield. Due to their versatility in replicating real-world process dynamics, predictive modeling is now extensively employed in biofuel research [35].

Machine learning (ML) offers a superior alternative to conventional RSM and OFAT techniques for managing the complex, non-linear relationships in biodiesel production systems [35]. A wide range of ML models, including ANN, ANFIS, ELM, SVM, KRR, and XGBoost, are now routinely used to forecast and optimize biodiesel yields, with algorithms like ANN and ensemble methods consistently providing higher accuracy [36]. However, existing studies typically focus on one- or two-ML techniques without broader comparative analysis, and most predictive models lack interpretability. While explainable artificial intelligence (AI) tools such as SHAP reveal how individual variables influence overall model performance, their application in biodiesel production modeling remains largely unexplored. Therefore, a gap exists in integrating dual waste feedstocks, composite biowaste-derived catalysts, multiple advanced ML models, and explainable analysis to improve both predictive accuracy and process understanding.

Following the prediction phase, optimizing parameters is crucial to maximize system efficiency. Because traditional tools like RSM are limited, nature-inspired heuristics such as GA, ACO, and MRFO are often combined with machine learning models [37–39]. Among these, MRFO is notable for its high performance in complex optimization tasks, inspired by the chain,

cyclone, and somersault feeding behaviors of manta rays [40].

Although periwinkle and coconut shells have been individually explored as sustainable feedstocks for solid catalyst synthesis, previous formulations using these individual feedstocks lacked sufficient bifunctional capabilities and stability. This has led to the use of less efficient, two-stage reactions for biodiesel synthesis. A thorough review of existing research indicates that periwinkle and coconut shells have never been used together to synthesize a bifunctional catalyst. Combining these complementary feedstocks offers an innovative approach to creating a bifunctional catalyst, leveraging coconut shell's high carbon content, low ash, and strong mechanical strength as a solid acid support [41]. Additionally, periwinkle shell ash contains high CaO content (up to approximately 93%), providing strong basicity for transesterification [42–44]. Developing catalysts from these feedstocks is expected to generate a positive synergy. Periwinkles are a major dietary staple in Nigeria, consumed regularly across millions of households and in commercial seafood markets. However, while the meat is harvested for food, the shells are discarded as municipal solid waste. In Nigeria, approximately 12 million tonnes of mixed agricultural waste shells (including periwinkle shells) are generated and improperly disposed of annually [33]. This creates significant environmental issues, such as blocked drainage systems, unsanitary heaps in local markets, and public health concerns [33,45]. Driven by increasing domestic consumption and industrial processing for coconut water and oil, large quantities of coconut shells are also generated daily as municipal waste. In Nigerian markets and processing centers, these non-degradable shells are typically accumulated in heaps or disposed of through open-pit burning, causing substantial particulate air pollution and environmental management problems [32]. Redirecting both periwinkle and coconut shell waste streams into biodiesel catalysts allows biorefineries to acquire highly functional raw materials at zero procurement cost. This approach directly addresses municipal solid waste management challenges across both coastal and terrestrial ecosystems in Nigeria.

This study introduces a novel approach for biodiesel synthesis through the synergistic valorization of dual waste feedstocks (waste cooking oil and waste animal fat) and a composite heterogeneous catalyst derived from coconut shell and periwinkle shell wastes. This work combines Box–Behnken experimental design with advanced

machine learning models (ANN, SVR, KRR, and XGBoost) to develop high-accuracy predictive tools for biodiesel yield. The process was further optimized using the MRFO algorithm. Additionally, SHAP-based feature importance analysis was employed to interpret nonlinear parameter interactions, while catalyst reusability studies validate the practical stability of the developed biowaste catalyst. Integrating eco-friendly catalyst production from waste materials with interpretable AI modeling represents a significant step toward smarter, greener biodiesel production.

2. Materials and Methods

2.1. Materials

All bio-based feedstocks were collected from various sources within Benin City, Nigeria, including waste cooking oil from a bean cake seller, fresh animal fat from the UBTH Cooperative abattoir, periwinkle shells from Uselu Market, and coconut shells from Ekosodin.

Additionally, the study utilized analytical-grade reagents, specifically benzene (99.99%), ethanol (99.99%), methanol (99.99%), copper nitrate (99%), and potassium hydroxide pellets (85%).

2.2. Methods

2.2.1. Oil feedstock and catalyst pretreatment

The collected animal fat was meticulously washed with tap water to eliminate residual blood and other impurities. Subsequently, it was cut into smaller fragments and subjected to slow heating in an oven at 60°C to facilitate melting. The liquefied fat was filtered using muslin cloth to remove any remaining particulates. Solid impurities were filtered from the WCO, which was then dehydrated by heating at 105°C for 2 hours. Following pretreatment, both feedstocks were preserved in separate airtight storage containers prior to use. Surface contaminants were removed from the waste periwinkle and coconut shells by rinsing with tap water. The cleaned biomass materials were then sun-dried for several days until completely dehydrated. The dry periwinkle shells were then processed using a mechanical grinder into powder form. Subsequently, a 250 µm (0.25 mm) sieve was used to sieve the powdered product. The resultant powdered material was then stored in an airtight jar.

2.2.2. Carbonization of coconut shells and Biochar Activation

The carbonization of the coconut shell was performed following the procedure described by

Osagiede and Aisien [20, 46], with slight adjustments to the operating conditions. The sieved coconut shell was carbonized at 700°C for 4 hours within a muffle furnace and subsequently cooled. For chemical activation, 5 g of coconut shell biochar (CS-BC) was stirred in 100 mL of 2 M KOH solution for 2 hours at ambient temperature. The resulting mixture was filtered and washed repeatedly until it reached a neutral pH. The sample was then dried at 105°C until fully dehydrated and stored in a cool, dry place.

2.2.3. Calcination of periwinkle shells

Sieved periwinkle shell powder (250 µm) was calcined at 900°C for 4 hours in a muffle furnace. After cooling overnight, the calcined periwinkle shell (CPS) was transferred to an airtight jar for storage.

2.2.4. Bifunctional catalyst preparation

The synthesis relied on CS-BC and calcined periwinkle shells as key precursors, using a wet impregnation technique adapted from the method described by Abdullah et al. [47].

Copper nitrate (5 wt%) and calcined periwinkle shells (30 wt%) were measured relative to the total weight of the activated CS-BC. The copper nitrate

was first dissolved in excess distilled water to ensure a homogeneous solution. Subsequently, the activated biochar and calcined periwinkle shells were introduced into the solution. The mixture was subjected to vigorous stirring for 6 hours at room temperature to facilitate the even distribution of the calcined periwinkle shell and the metal precursor onto the support surface.

2.2.5. Catalyst characterization

Comprehensive characterization of the catalyst and its precursor materials was conducted using SEM-EDX for surface topology and elemental composition, FTIR for functional group identification, and XRD (Cu-K radiation) for crystal phase determination. Thermal stability and surface area metrics were subsequently evaluated using DTA and the BET method, respectively. The Hammett indicator technique was employed to measure catalyst basicity.

2.2.6. Blending and characterization of oils

The oil blend was formulated using the optimized ratio of 57.5% WCO to 42.5% AF, as previously reported [16]. The physicochemical properties of the oils before and after the blend, determined using ISO standard methods, are shown in Table 1.

Table 1. Physiochemical properties of WCO, AF, and the blend

S/N	Properties	Test Standard	AF	WCO	AF-WCO Blend
1.	Acid Value (mg KOH/g)	EN 14104	1.01	6.10	4.72
2.	Free fatty Acid (%)	-	0.52	3.11	2.36
3.	Density (kg/m ³)	EN ISO 12185	1060	950	910
4.	Saponification Value (mg KOH/g)	ISO 3657	156.1	244.8	167.2
5.	Viscosity @ 40 °C (mpas).	EN ISO 3104	4.74	3.33	4.05
6.	Peroxide value (meq/kg)	ISO 3960	0.32	3.94	0.68

2.2.7. Experimental Design and Data

Preprocessing

The Box-Behnken Design (BBD) of RSM was utilized to generate the design matrix for the transesterification process, incorporating four independent factors: Reaction temperature (RT), Catalyst loading (CL), Reaction time (Rt), and Methanol-to-Oil Ratio (MTOR). The ranges of values chosen for the factors, depicted as coded and actual values, are illustrated in Table 2.

Design Expert 13.0 software generated the experimental design based on the principle of randomization to reduce the influence of residual variance on the target response parameters. The biodiesel yield was the primary response analyzed. According to the design, twenty-

nine experimental runs were performed in a randomized sequence.

Before training the models, all input variables were feature-scaled using the StandardScaler from the Scikit-Learn library (version 1.5.2) to bring them within a normal distribution. Feature scaling was applied to eliminate magnitude-based bias across variables and to improve training convergence.

Table 2. Experimental design based on BBD

Factors	Symbol	values		
		low	0	high
RT (°C)	Z ₁	50	65	80
CL (wt%)	Z ₂	3	6.5	10
Rt (min)	Z ₃	60	105	150
MTOR	Z ₄	3	8.5	14

2.2.8. Biodiesel production and characterization

The transesterification of the oil blend was carried out using a modified one-step protocol [25].

The feedstock was heated in a 250 mL flask mounted with a magnetic stirrer. Upon reaching the target temperature, a predetermined amount of methanol was introduced into the flask, mixed for 5 minutes, and combined with the bifunctional catalyst. Following the reaction period, centrifugation was used to remove the suspended solids, and the liquid phase was allowed to settle overnight in a separating funnel. After discarding the lower glycerol-rich fraction, the raw biodiesel was rinsed three times with warm deionized water, dried of residual moisture, and bottled for subsequent characterization. The yield was determined using Equation (1).

$$\text{yield (\%)} = \frac{\text{weight of the biodiesel (g)}}{\text{weight of oil used (g)}} \times 100 \quad (1)$$

2.2.9. Machine learning model development

Experimental datasets were processed, modeled, and optimized using Python (v3.11.9) in Visual Studio Code (v1.101) on an Intel Core i7 Windows 11 system (16 GB RAM). Primary data handling relied on NumPy (v2.0.2) and Pandas (v2.2.3), with Matplotlib used for graphical plotting. Four predictive models were trained on the experimental results: SVR and KRR (Scikit-learn v1.5.2), ANN (TensorFlow v2.19.0), and XGB (XGBoost v2.1.4). Data were split into an 80:20 training-to-testing ratio (random_state=42). To ensure zero data leakage, scaling transformations were trained strictly on the training data prior to transforming the test set. Hyperparameter tuning for all machine learning models was performed through Bayesian optimization using the Optuna library (version 4.2.1), a flexible and efficient hyperparameter optimization framework. Unlike grid or random search methods, Bayesian optimization leverages information from prior evaluations to construct a surrogate model that approximates the correlation between hyperparameters and the objective function's performance. This model guides the selection of subsequent hyperparameter configurations in a more informed and efficient manner, thereby accelerating convergence toward optimal solutions [84]. Each model's objective function was defined based on the R2 score on the test set, and trials were executed over a well-defined search space for each algorithm. The best performing set of hyperparameters was then used for final training and evaluation.

2.2.10. Artificial neural network modelling

Modeled after human brain neurology, Artificial Neural Networks (ANNs) are particularly effective at predicting complex, non-linear optimization outcomes [48]. They consist of interconnected processing elements known as neurons. These neuron structures work together in a synchronized manner to address and solve complex problems [49]. ANNs have been widely applied in modeling process variables in biofuels synthesis, significantly minimizing the trial-and-error approach required by traditional experimental methods [38].

The ANN features a fully connected feedforward design with a four-neuron layer (one for each process variable) and three hidden layers. As shown in Equation 2, each neuron generates an output (z) by summing the products of inputs (x_i) and weights (w_i), plus a bias (b).

$$z = \sum_{i=1}^n x_i w_i + b \quad (2)$$

Each hidden layer employs an activation function to map inputs to the corresponding outputs. Overfitting was managed by incorporating dropout layers into the network. Model optimization involved comparing SELU and ReLU activation functions, with the final architecture utilizing a single output neuron to predict biodiesel yield based on transformed representations from the hidden layers. As shown in Equations (3) and (4), the network was iteratively trained by applying gradient descent to adjust weights, scaled by the learning rate (λ), to minimize the loss function (ℓ).

$$\ell = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (3)$$

$\hat{y}_i$ = model's predicted output.

$$w_{t+1} = w_t - \lambda \frac{\partial \ell}{\partial w_t} \quad (4)$$

2.2.11. Support vector regression

SVM is among the widely used techniques for non-linear regression analysis [50]. The method is unique in that it determines the most effective hyperplanes for separating data points, making it a practical tool in machine learning. SVR is a robust supervised machine-learning technique widely applied to regression and predictive modeling tasks [35]. As expressed in Equation (5), the model determines a function, y , that predicts the target values within a specified error margin (ϵ), while maintaining a relatively simple model structure.

SVR aims to minimize the cost function shown in Equation (6).

$$y = wx + b \quad (5)$$

$$\min_{w,b,\xi_i,\xi_i^*} \frac{1}{2} w^T w + K \sum_{i=1}^n \xi_{i_i} + \xi_{i_i}^* \quad (6)$$

2.2.12. Kernel ridge regression

KRR models combine ridge regression with kernel methods to model non-linear relationships between features and targets. It employs regularization to prevent overfitting, making it suitable for moderate or small datasets [35]. The model's formulation is shown in Equation 7, where the constituent term is governed by Equation (8).

$$\arg \min \frac{1}{m} \sum_{i=1}^m \|f_i - y_i\|^2 + \lambda \|f\|_H^2 \quad (7)$$

$$f_i = \sum_{j=1}^m \alpha_j (x_j, x_i) \quad (8)$$

Where $\|f\|_H$ is the Hilbert normed space.

The RBF and linear kernel types were explored, and the hyperparameter space included the regularization parameter alpha, the kernel coefficient gamma, the polynomial degree (for the polynomial kernel), and the offset term coef0. Hyperparameter optimization was performed using the Optuna library to identify the configuration that maximized predictive performance.

2.2.13. Extreme gradient boosting

The XGB algorithm has gained prominence over the years due to its robustness in capturing nonlinearities and complex feature interactions. For a given step in time (t), the prediction function is defined by Equation (9).

$$f_i^{(t)} = \sum_{k=1}^t f_{k_i}(x_i) = f_i^{(t-1)} + f_i(x_i) \quad (9)$$

$f_i(x_i)$, $f_i^{(t)}$, $f_i^{(t-1)}$ and x_i denote the base learner, current prediction, previous prediction, and input data at step t, respectively. To mitigate overfitting in the XGBoost model, specific equations are employed to evaluate how well the model fits the original function, as illustrated by Equation (10).

$$obj^{(t)} = \sum_{k=1}^n l(\bar{y}_i, y_i) + \sum_{k=1}^t \Omega(f_i) \quad (10)$$

Where l denotes the loss function, n the sample size, and Ω the regularization term as defined in Equation (11).

$$\Omega(f) = \gamma T + \lambda \|\omega\|^2 \quad (11)$$

Hyperparameter tuning involved the number of estimators, maximum tree depth, learning rate, regularization parameters, and sampling ratios. Optimization was conducted using the Optuna library to minimize overfitting and maximize model generalization.

2.2.14. Model assessment

Model efficacy was evaluated using multiple complementary metrics. Goodness of fit and predictive errors were measured with R2 and (MSE and RMSE), respectively. This multi-metric approach aimed to ensure that the model is both accurate and generalizable.

In addition, the absolute average deviation (AAD) was included to provide a measure of average error magnitude that is less sensitive to outliers. AIC was also employed to assess the balance between model fit and complexity, supporting the selection of simpler models that still perform well on new, unseen data. This multi-metric approach enabled a comprehensive evaluation of each model's performance from multiple perspectives.

2.2.15. Integration of best model with manta-ray foraging optimization

The best model was applied as a surrogate to maximize biodiesel yield. The MRFO algorithm was chosen for its effective global search capabilities [39]. Search parameters were constrained by the experimental bounds of the four input features. MRFO settings such as population size, iteration count, and somersault range were fine-tuned. This process was designed to accelerate convergence without trapping the model in local optima.

Among the three foraging strategies embedded in MRFO, the somersault foraging phase is important for intensifying the search around the best-known solution. This phase is expressed as shown in Equation 12 [39].

$$X_i^{t+1} = X_i^t + S \cdot (r_1 \cdot X_{best}^t - r_2 \cdot X_i^t) \quad (12)$$

Where X_i^t represents the current i^{th} solution at iteration t, X_{best}^t is the global best solution at iteration t, S is the somersault factor (user-defined), and r_1 and r_2 are random values in the range [0,1]. This mechanism encourages candidate solutions to explore the region around the best solution while maintaining diversity in the population.

The MRFO algorithm iteratively searched the input space to identify the configuration that maximized the predicted yield from the surrogate model, demonstrating its utility for guiding optimal biodiesel production conditions.

2.2.16 SHAP-based model interpretability

SHAP was employed to enhance the explainability and interpretability of the top model. Grounded in cooperative game theory, this unified framework measures feature contributions to specific predictions [51]. It effectively quantifies how each input impacts individual outputs. This was essential for validating the model's reasoning and ensuring alignment with established domain knowledge in biodiesel production. Global feature importance was assessed using SHAP's beeswarm plot, which ranks input variables based on the magnitude and direction of their average impact across all predictions [52]. This visualization enabled a holistic understanding of which factors most strongly influenced biodiesel yield. Local explanations for individual predictions were provided via waterfall plots, which measure each feature's additive impact on a single prediction. This type of plot is widely recognized for offering clear insights into how feature values push the model's output above or below its baseline [53]. Together, the combination of global (beeswarm) and local (waterfall) SHAP analyses enabled validation of the model's reasoning against domain knowledge and supported interpretability in the context of biodiesel yield optimization.

3. Results and discussion

3.1. Catalyst characterization

3.1.1. SEM-EDX analysis

The SEM images and the EDX results are presented in Figures 1 and 2, respectively. Figure 1(a) shows the surface morphology of CS-BC, providing insights into its structural characteristics. As observed, the surface pores are progressively open and distributed across both the surface and the cavity walls, highlighting its porous structure. The high porosity of the precursors is beneficial, as it enables the efficient attachment of active sites onto the catalyst surface during the impregnation process [20]. Paputungan et al. [54] reported similar results in their study focusing on the adsorption capacity of activated carbon derived from coconut shells.

The surface morphology of calcined periwinkle shells is presented in Figure 1(b), offering detailed microstructural features. It reveals a highly porous, rough, and fractured microstructure with significant cracking, agglomeration, and irregular grain sizes. The observed porous network is consistent with previous studies on biogenic calcium oxides (CaO), where calcination of shells leads to decarbonation-induced porosity and surface roughening, thereby enhancing adsorption and catalytic properties [55, 56]. The presence of

microcracks and voids aligns with reports on thermal stress and CO₂ evolution during high-temperature calcination, which contribute to brittleness [57]. Additionally, agglomerated clusters suggest localized sintering, a phenomenon observed in similar biomaterials calcined above 800°C [58]. This microstructural characteristic enhances potential applications in catalysis, where high surface area and CaO content are desirable [56].

Figure 1(c) displays the composite bifunctional catalyst which reveal a highly porous structure with rough, irregular morphology and dispersed white particles, likely representing copper deposits and CaO-rich phases. The presence of pores in the material suggests a significant surface area, crucial for catalytic applications. Similar biochar-based catalysts exhibit enhanced adsorption capacities and well-distributed dopants, improving active site availability [59]. The observed CaO-rich regions align with literature on calcined shell-based catalysts, which enhance basicity for transesterification reactions [60]. Additionally, the agglomeration of copper nanoparticles, seen in some regions, supports previous findings that metal-doped biochar improves catalytic efficiency in biodiesel synthesis [61].

The EDX results shown in Figure 2 provide insights into their elemental composition. Figure 2(a) reveals that CS-BC contains metals such as potassium and calcium in small quantities. Figure 2(b) indicates that waste periwinkle shells primarily contain calcium, iron, aluminum, and magnesium. The presence of highly reactive metals, including iron, aluminum, calcium, copper, magnesium, and potassium, in the composite bifunctional catalyst, as depicted in Figure 2(c), contributes to its enhanced catalytic activity.

3.1.2. FTIR Analysis

Figure 3 presents the FTIR spectra that identify the precursors and catalyst surface functional groups, chemical composition, and surface traits. The coconut shell biochar spectrum in Figure 3(a) displays aromatic C=C vibrations (1600–1400 cm⁻¹), oxygenated groups (C=O at 1632 cm⁻¹), and C–O stretching (1300–1000 cm⁻¹). These features indicate partial graphitization and an oxygen-rich surface. Together, they increase surface area and enhance reactant adsorption [62]. Figure 3(b) highlights strong Ca–O stretching below 600 cm⁻¹, reduced carbonate peaks, and the loss of organic functional groups. This confirms the successful conversion of CaCO₃ to CaO, a highly active base catalyst for transesterification [63, 64]. Finally, Figure 3(c) reveals Cu–O bands at 600–

500 cm^{-1} , shifted C=O and C–O peaks (1000–1100 cm^{-1}), and decreased aliphatic C–H intensity (2900–2850 cm^{-1}). These shifts confirm Cu^{2+} incorporation, which introduces Lewis acid sites that work synergistically with CaO to boost transesterification efficiency [65, 66]. These spectral modifications confirm that the composite

catalyst combines basic (CaO) and acidic (Cu^{2+}) active sites with a high-surface-area biochar support, optimizing it for efficient biodiesel synthesis by promoting both triglyceride conversion and an enhanced reaction process.

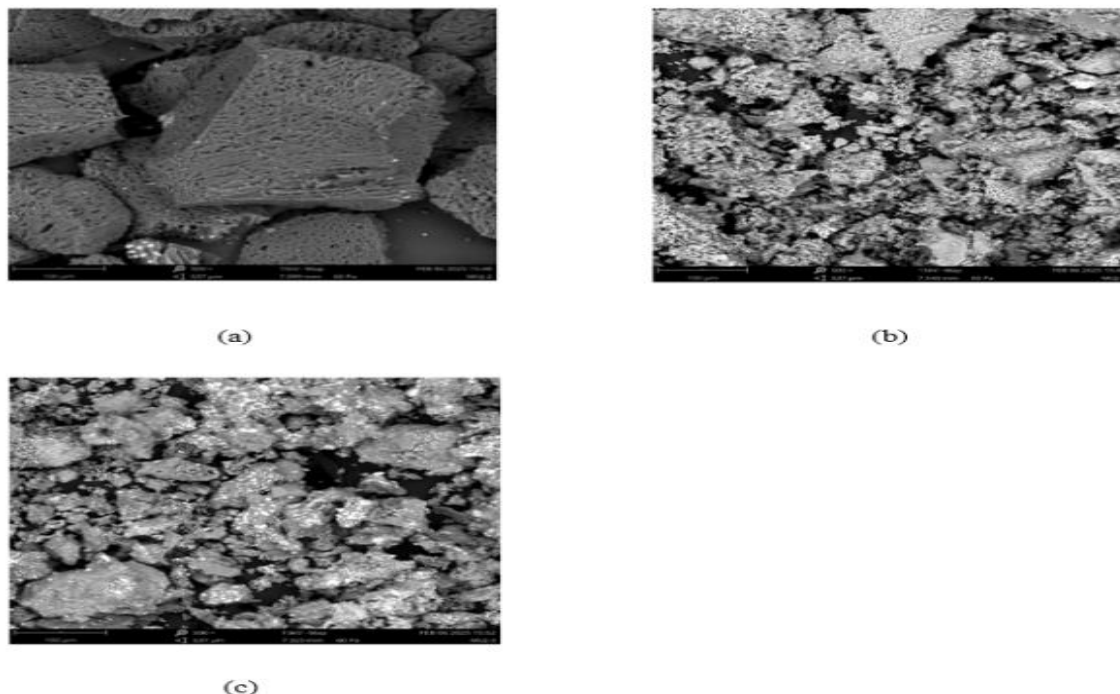


Figure 1. SEM micrograph of (a) CS-BC, (b) CPS and, (c) Bifunctional catalyst (Cu-CS-BC/CPS)

3.13. TGA/DTA Analysis

Figure 4 (a), (b), and (c) show the TGA/DTA analysis of CS-BC, calcined periwinkle shell and composite catalyst respectively, revealing distinct thermal decomposition behaviors. The activated carbon shows high thermal stability, with minor weight loss below 150 $^{\circ}\text{C}$, followed by gradual decomposition from 250–600 $^{\circ}\text{C}$, mainly due to residual organic matter oxidation, stabilizing beyond 600 $^{\circ}\text{C}$, indicating a high fixed carbon content suitable for adsorption applications [67]. The periwinkle shell exhibits a two-stage weight loss: initial moisture removal below 200 $^{\circ}\text{C}$, followed by major decomposition between 600–800 $^{\circ}\text{C}$, confirming CaCO_3 breakdown into CaO , a process consistent with biogenic CaCO_3 transformations [64, 68]. The composite exhibits multi-step degradation, with copper nitrate decomposition around 250–350 $^{\circ}\text{C}$, accelerating the carbon oxidation process, evidenced by a peak near 300 $^{\circ}\text{C}$ and a broader peak beyond 500 $^{\circ}\text{C}$,

confirming enhanced thermal stability and catalytic potential [69]. These thermal profiles suggest that the catalyst holds promise for catalytic applications.

3.14. Brunauer-Emmett-Teller analysis

The BET analysis of the precursors (CS-BC and CPS) and the final synthesized catalyst was performed using N_2 adsorption-desorption isotherms. The Specific Surface Area (SSA), Total Pore Volume (TPV), and Mean Pore Diameter (MPD) are presented in Table 3.

Table 3: BET results of CS-BC, CPS and the final synthesized catalyst

Material	SSA (m^2/g)	TPV (cm^3/g)	MPD (nm)
CS-BC	256.5	0.38	3.22
CPS	28.91	0.04	15.2
Catalyst	143.8	0.26	4.61

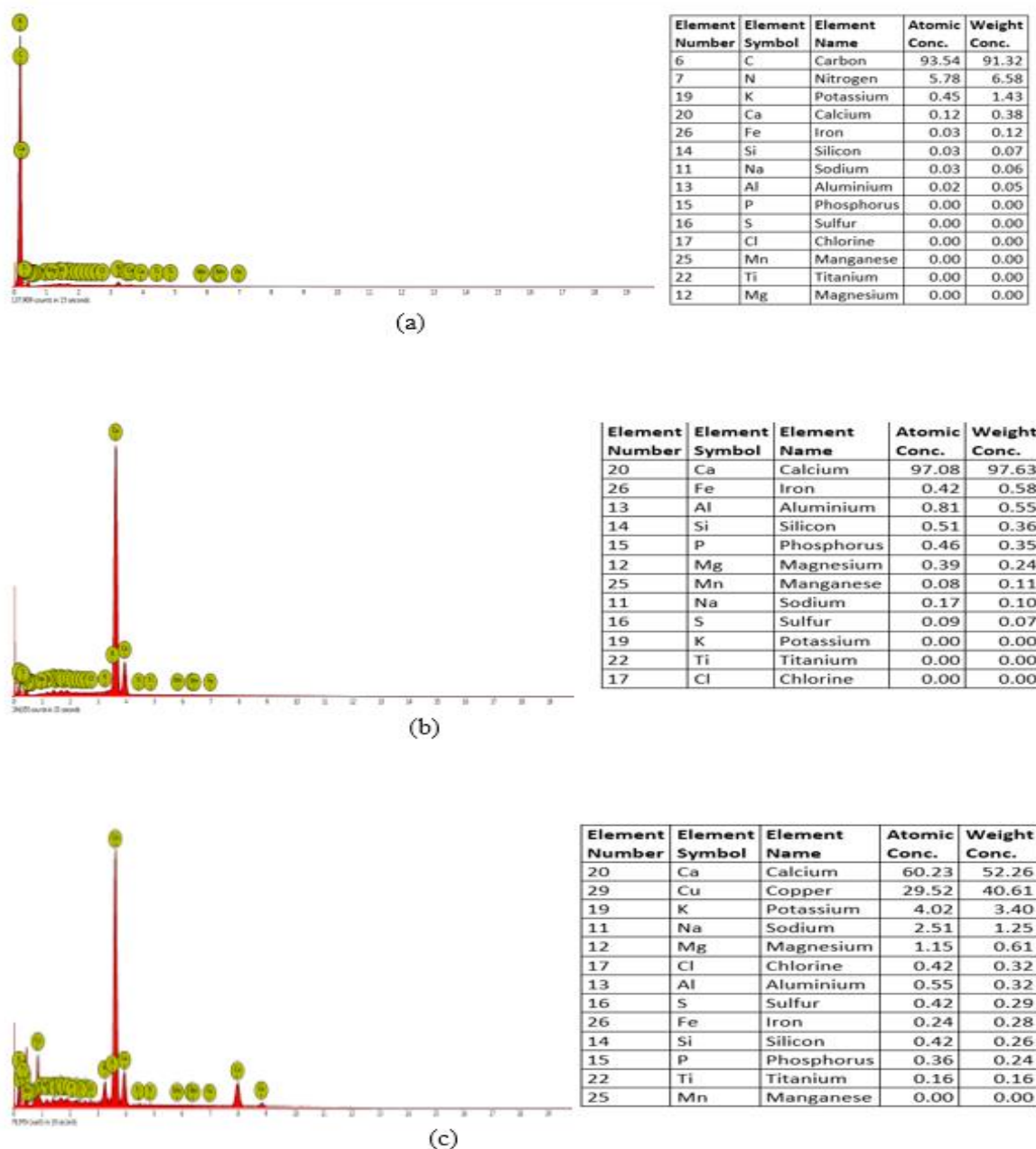


Figure 2. EDX analysis of (a) CS-BC, (b) calcined periwinkle shells and, (c) bifunctional catalyst (Cu-CS-BC/CPS)

The CS-BC exhibited a high SSA of 256.5 m²/g and a large TPV of 0.38 cm³/g, with an MPD of 3.22 nm. This confirms that CS-BC functions as a highly porous, mesoporous carbon carrier suitable for anchoring active chemical species. In contrast, the calcined periwinkle shell (CPS) showed a significantly lower SSA of 28.91 m²/g and a minimal TPV of 0.04 cm³/g, accompanied by a larger MPD of 15.2 nm. Upon impregnating the CS-BC framework with CPS and copper species to formulate the composite catalyst, the SSA decreased from 256.5 to 143.8 m²/g, and the TPV decreased from 0.38 to 0.26 cm³/g. This reduction in SSA and TPV is a classic indicator of successful

composite formation. Active metal oxides (CaO and CuO) penetrate and deposit inside the micro- and mesoporous channels of the CS-BC matrix, causing partial pore blockage and spatial filling of the carbon pores. Although impregnation lowered the values of these properties, the resultant values for the catalyst remained adequate for good catalytic performance. Similar characteristics have been reported for biodiesel catalysts derived from cow horn [19] and rubber seed eggshells [20].

3.15. Catalyst basicity analysis

The Hammett indicator titration revealed that the synthesized Cu/CPS-BC catalyst possesses a total

basic site density of 1.84 mmol/g at a basic strength range of $8.2 \leq H_{\text{b}} \leq 15$. This substantial basicity is primarily attributed to the thermal conversion of CaCO_3 in the periwinkle shells during calcination at 900 °C, which yields highly reactive CaO basic sites. A basicity value of 1.84 mmol/g compares

favorably with several reported heterogeneous biochar-supported catalysts in the literature [87–89]. This confirms that the porous coconut shell biochar (CS-BC) successfully trapped a high dispersion of CaO without severe agglomeration [20].

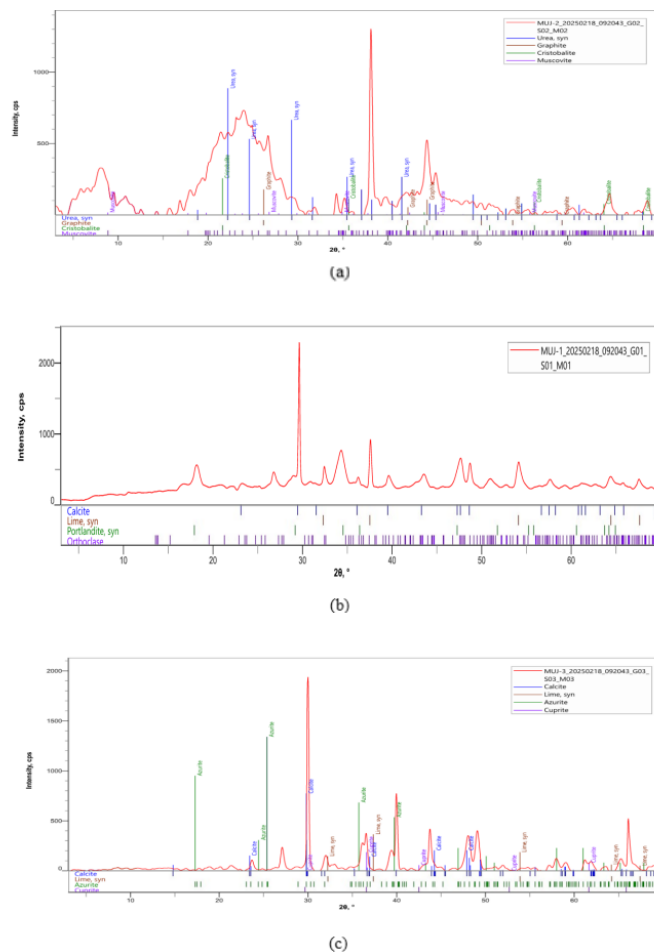


Figure 3. FTIR analysis of (a) CS-BC, (b) calcined periwinkle shell and, (c) bifunctional catalyst

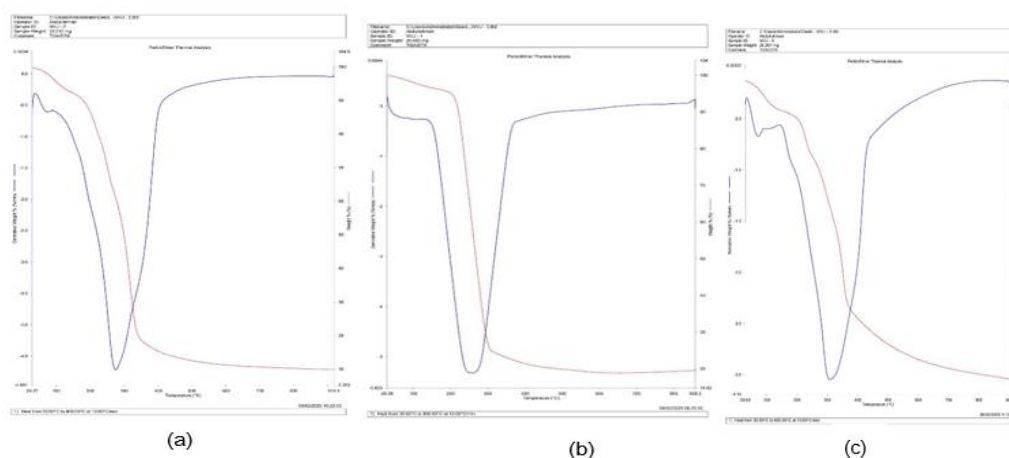


Figure 4. TGA/DTA of (a) CS-BC, (b) calcined periwinkle shell and, (c) bifunctional catalyst

3.2. Machine learning modelling

The machine learning models were developed using data generated from the biodiesel production experiments, and their hyperparameters were optimized with Optuna's Bayesian optimization framework. This approach enabled an efficient and informed exploration of the hyperparameter space by leveraging past trial results to guide subsequent evaluations. The performance of each model, based on its optimized hyperparameters, was evaluated using statistical metrics as presented in Table 4.

All four machine learning models exhibited strong predictive capabilities for modeling biodiesel yield. The coefficient of determination (R^2) on the test set exceeded 0.8 across all models, reflecting good generalization performance [70]. Among them, the Support Vector Regression (SVR) model achieved the highest test R^2 , indicating strong predictive alignment with unseen data. However, its relatively high error metrics (MSE, RMSE, and AAD) suggest greater deviation from actual values, limiting its overall reliability. The Kernel Ridge Regression (KRR) model also demonstrated solid predictive ability, with a test R^2 of 0.9182 and moderate error metrics. While its performance was stable, it did not surpass the top models in either accuracy or error minimization. Nevertheless, its relatively low AIC (which assesses the balance between model fit and complexity) and consistent R^2 scores across training and test sets indicate a well-regularized model that avoided overfitting. The ANN model achieved outstanding training efficiency and recorded the lowest overall error. Taking all evaluation metrics as displayed in Table 4 and the visualizations in Figure 5 into account, the XGB model was identified as the most robust and well-rounded. It maintained strong

metrics on the full dataset. However, its test R^2 dropped to 0.8405, the lowest among all models, suggesting potential overfitting and reduced generalizability. ANNs use backpropagation through interconnected layers to learn patterns in the data. When the dataset is small, as is common with experimental designs such as a Box–Behnken Design with 29 runs, the model may have too many parameters relative to the available data. This can make the model more prone to overfitting and reduce its ability to perform well on new data [85]. Therefore, the other statistical metrics cannot serve as reliable benchmarks for comparing this model with the others. On the other hand, the Extreme Gradient Boosting (XGB) model provided the most balanced performance. It achieved a high test R^2 , indicating accurate and consistent predictions. Its AIC was also favorably low. Lower or more negative AIC values indicate a better model due to their favorable trade-off between predictive power and computational complexity. XGBoost recorded the lowest AIC value of -75.2046 , compared with -56.1301 for SVR and -60.3008 for KRR. This further suggests that XGBoost provided the best overall fit while maintaining relatively low model complexity. This reflects a good balance between model complexity and fit. Parity plots in Figure 5(a–d) show the predicted versus actual values. Data points cluster tightly around the 45° reference line, signaling high accuracy. Table 5 also compares actual versus predicted values. The strong alignment validates model performance.

generalization capability, low prediction errors, and efficient complexity, making it the most suitable model for subsequent optimization and interpretability analyses.

Table 4. Statistical assessment of model predictions

Parameter	ANN	SVR	KRR	XGB
Train R^2	0.9965	0.8861	0.9071	0.9570
Test R^2	0.8405	0.9329	0.9182	0.8989
Full data R^2	0.9641	0.8978	0.9114	0.9470
MSE	0.0359	0.1022	0.0886	0.0530
RMSE	0.1894	0.3198	0.2976	0.2301
AAD	0.1109	0.2108	0.2371	0.1794
AIC	-80.5202	-56.1301	-60.3008	-75.2046

Several studies have utilized XGB for transesterification modeling. Suvarna et al. [71] predicted and optimized biodiesel fuel properties with XGB, achieving high R^2 scores for CN and CFPP among the different ML models used. Şahin and Torun [72] also employed three machine learning models (ANN, Random Forest, and XGB) to explore the viability of using pumpkin seed oil

as a biodiesel feedstock, and the XGB model emerged as the most accurate for predicting the performance and emissions of the fuel blend. These studies demonstrate the reliability of the XGB model, particularly for datasets with limited samples, similar to this study, compared to other ML variants.

Table 5. Comparison of Machine learning model's prediction with experimental values

Run no	Input Features					Response (Biodiesel yield (%))			
	Reaction Temperature (c)	Catalyst Loading (wt%)	Reaction Time (min)	Methanol – oil ratio	Experimental yield	SVR prediction	KRR prediction	ANN prediction	XGB Prediction
1	65	6.5	60	14.0	69.12	69.87	70.49	69.22	69.82
2	65	10.0	105	14.0	70.78	70.02	69.93	70.39	70.43
3	80	6.5	105	14.0	66.98	65.61	64.77	66.06	67.46
4	65	10.0	60	8.5	76.23	75.48	74.54	75.84	75.72
5	50	10.0	105	8.5	69.21	69.96	70.13	68.76	69.00
6	65	6.5	105	8.5	76.70	77.45	76.86	76.77	77.82
7	80	6.5	60	8.5	76.12	75.37	74.90	76.14	74.29
8	65	3.0	105	14.0	74.68	74.38	74.99	75.17	76.34
9	50	6.5	105	3.0	66.01	68.45	68.56	66.03	68.18
10	50	3.0	105	8.5	76.21	75.46	75.62	75.96	76.18
11	65	3.0	150	8.5	79.20	78.45	77.98	76.92	79.35
12	65	10.0	150	8.5	77.10	76.35	75.14	77.06	76.62
13	80	3.0	105	8.5	72.21	72.96	73.92	72.79	72.39
14	50	6.5	60	8.5	63.99	65.09	66.08	64.30	65.74
15	65	6.5	105	8.5	76.80	77.45	76.86	76.77	77.82
16	50	6.5	105	14.0	65.89	65.21	66.27	66.07	67.92
17	65	6.5	150	14.0	69.01	69.76	70.47	71.44	69.51
18	65	10.0	105	3.0	74.85	74.10	74.12	74.80	74.23
19	65	6.5	150	3.0	71.3	72.05	72.69	71.39	71.96
20	80	10.0	105	8.5	60.31	67.32	64.18	60.77	62.94
21	65	6.5	105	8.5	76.97	77.45	76.86	76.77	77.82
22	80	6.5	150	8.5	68.50	68.54	67.96	68.69	68.54
23	65	3.0	60	8.5	82.30	81.55	80.84	82.00	81.89
24	65	6.5	60	3.0	75.02	75.77	75.84	75.46	74.74
25	80	6.5	105	3.0	70.21	69.46	69.80	69.11	69.16
26	65	3.0	105	3.0	76.31	77.06	76.79	76.91	76.54
27	65	6.5	105	8.5	76.38	77.45	76.86	76.77	77.82
28	50	6.5	150	8.5	70.40	71.15	71.33	70.10	69.46
29	65	6.5	105	8.5	80.20	77.45	76.86	76.77	77.82

3.3. Response Surface plots

3D surface plots were used to analyze how input variables individually and interactively affect biodiesel yield. Figure 6(a) shows the joint effect of RT and CL. Yield increases as both parameters rise. It peaks broadly at 65–70 °C and 3–4 wt% CL. Beyond this region, the surface starts to flatten or slightly decline, indicating diminishing returns or possible inhibition effects at higher values of both variables. The contour projections support this, showing closely spaced lines near the lower ranges (indicating a steep gradient in yield improvement) and wider spacing at the top, reflecting yield stabilization. This suggests that excessively high temperature or catalyst loading does not significantly improve biodiesel yield and may even slightly reduce it. This aligns with studies that support the notion that exceeding optimal reaction conditions can negatively impact yield due to issues such as methanol evaporation at high temperatures or catalyst saturation effects at excessive loadings [73, 74].

Figure 6(b) presents the joint influence of RT and Rt on biodiesel yield. Yield initially rises with higher values for both parameters. An optimal region is reached around 65 °C and 100–110

minutes. Beyond this point, further increases in RT or Rt lead to a reduction in yield. This trend likely reflects thermal degradation of the product or methanol evaporation at higher temperatures, and possible side reactions or catalyst deactivation over extended reaction durations. Several studies have reported these findings [75, 76]. Figure 6(c) shows how RT and MTOR jointly affect the yield of biodiesel. An initial rise in yield is driven by increasing both variables. Peak yield is attained at moderate parameter levels. However, above the optimal points, the yield starts falling, indicating that excessive methanol or overly high temperatures may have adverse effects. This behavior is likely due to methanol evaporation at elevated temperatures and dilution effects at high methanol ratios which hinder the transesterification reaction [77]. Similarly, Figure 6(d) illustrates the joint effect of CL and Rt on biodiesel yield. Yield initially decreases as both parameters increase. A minimum value is reached at moderate levels of CL and Rt. However, beyond these mid values, further increase results in a significant increase in biodiesel yield. This trend suggests that insufficient catalyst or short reaction durations may limit the transesterification efficiency, while higher catalyst

concentrations and prolonged reaction times enhance conversion. This is likely caused by enhanced reactants contact and longer reaction time that allow the process to reach completion [78]. Figures 6(e) and (f) show similar trends with CL, MTOR and Rt. Similar results have also been reported by Enguilo et al. [79] who found that an

optimal MTOR of 12:1 and a CL of 5 wt.% yielded 90% methyl ester content using an iron and calcium oxide-based bifunctional catalyst with WCO. These findings emphasize that optimal conditions may lead to decreased yields hence the need for optimization of process parameters.

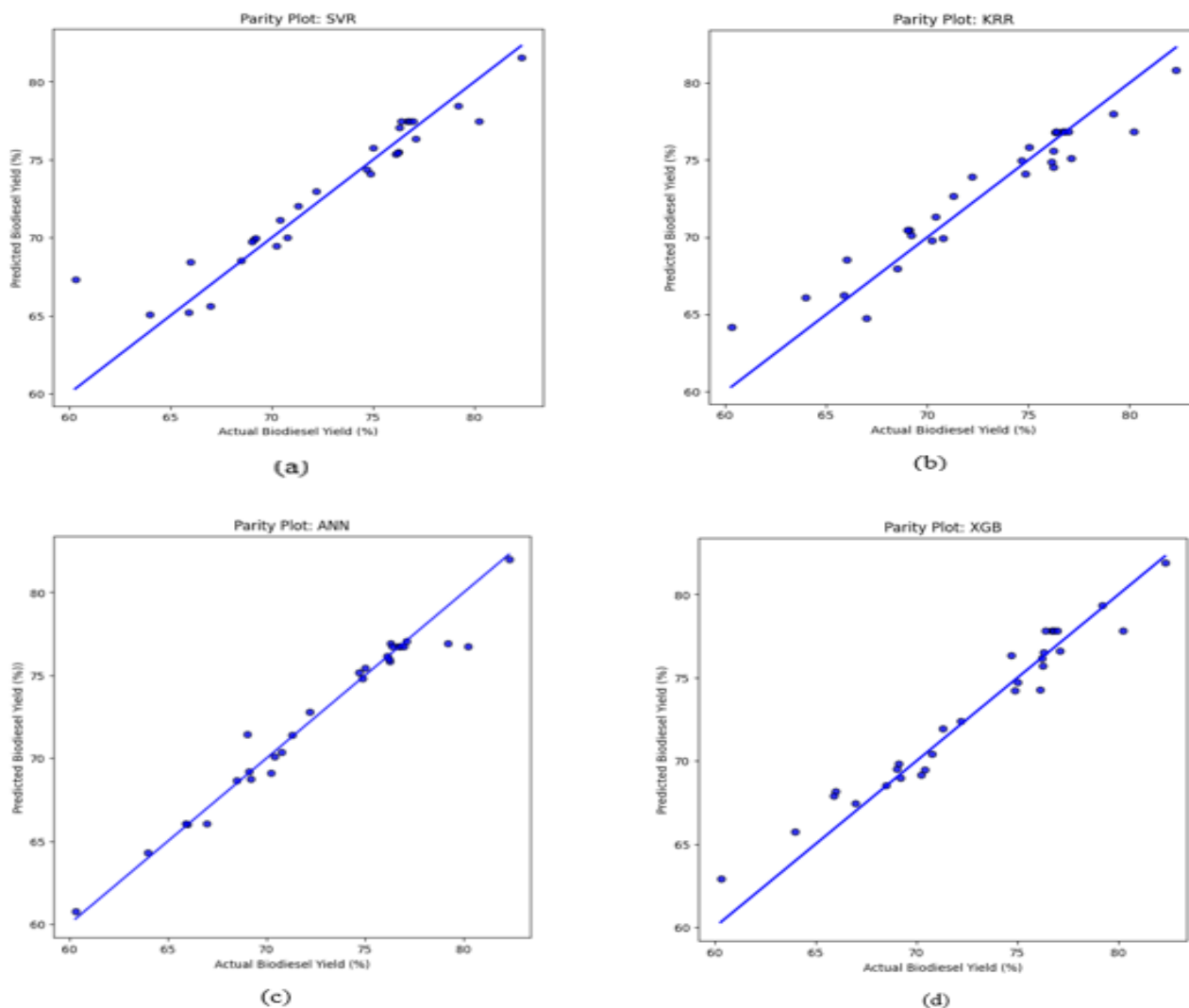


Figure 5. Parity plots showing (a) SVR, (b) KRR, (c) ANN, and (d) XGB

3.4 Optimization Process

Table 6 presents the hyperparameters selected for the MRFO algorithm. These parameters were applied in the optimization process and the results are shown in Table 7. The algorithm predicted a maximum biodiesel yield of 81.90%. The corresponding optimized conditions were 66 °C, 6.37 wt% catalyst, 104.61 minutes, and a 8.84 MTOR. This effectively mirrors the XGB model's best 81.89% prediction. This close alignment highlights the reliability and near-optimal

capability of the XGB model, validated further by MRFO's independent search. The minimal improvement suggests that the XGB-driven baseline was already situated near the global optimum. Validation of results was conducted through three independent experimental replicates performed using the optimized conditions. A mean biodiesel yield of $82.3 \pm 0.8\%$ was achieved. These results demonstrate strong alignment between predicted and actual values, showing a minimal percentage error of 0.49%.

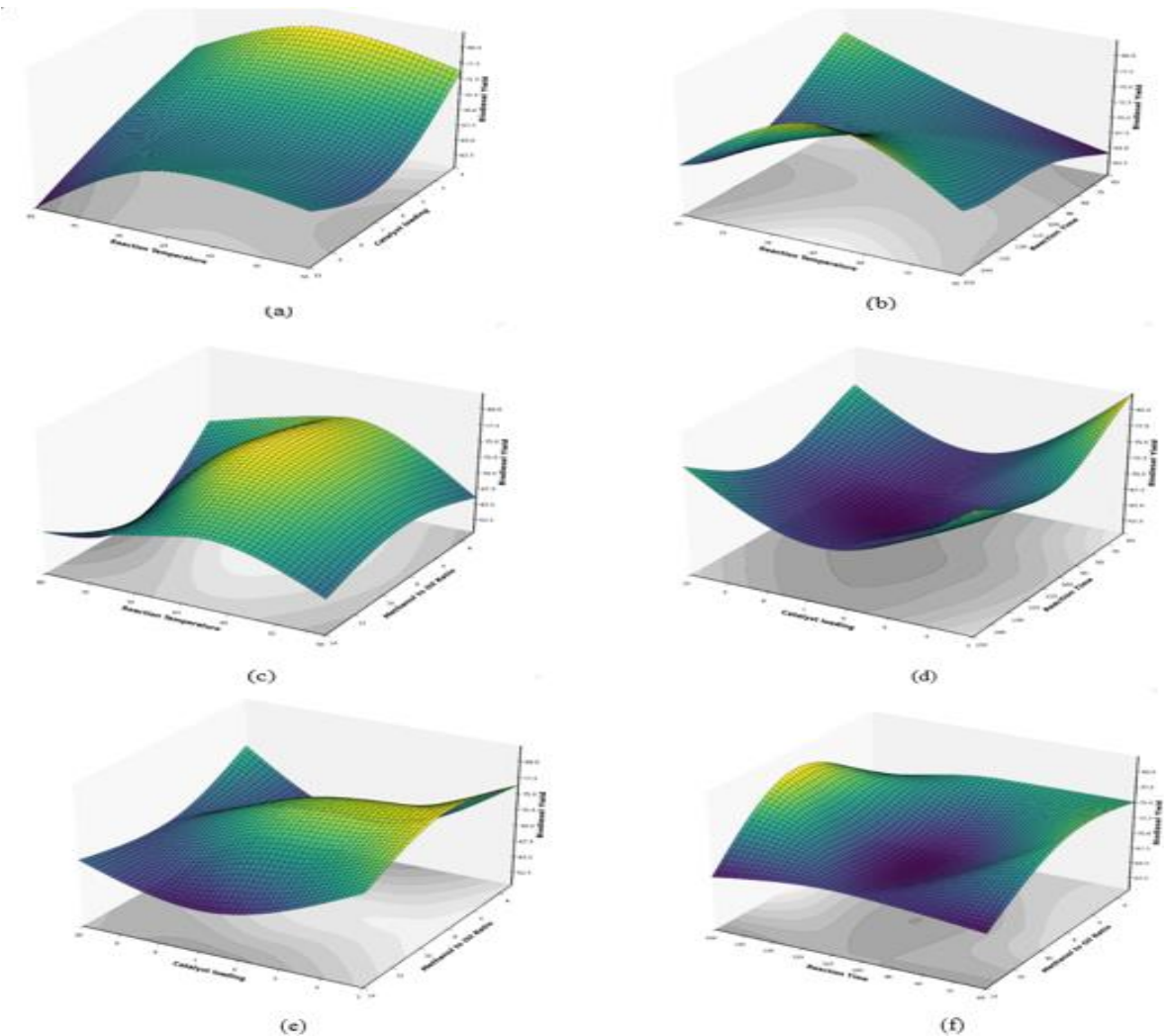


Figure 6. Plots showing the combining influence of (a) RT and CL, (b) RT and Rt, (c) RT and MTOR, (d) CL and Rt, (e) CL and MTOR, and, (f) Rt and MTOR on biodiesel yield.

When compared with benchmarks in the literature, this study’s results align with Abdulla et al. [80], who reported an 82.8% biodiesel yield at 59.4 °C and a 12:1 MTOR, and with the findings reported by Pranita et al. [81], which achieved an optimal yield of 82.79% for Kemiri Sunan oil using two-stage transesterification at 65 °C and a 6:1 methanol ratio. Table 8 shows how the results obtained in this study compare to some reported findings. Although the maximum biodiesel yield (82.3%) achieved in this investigation is slightly below the literature benchmarks of 82.8%–98%, this yield was obtained under less critical reaction conditions. Additionally, our newly formulated catalyst has demonstrated superior stability, with up to 97.1% activity retention after five cycles of reuse.

Table 6. Hyperparameters for MRFO algorithm

MRFO Hyperparameters	Final Optimized Value
Epoch	5
Population Size	10

Somersault Range	1.0
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3.5. Feature importance via SHAP

The input features were ranked based on their output influence using SHAP ranking and beeswarm plots. Global interpretations of feature impacts are enabled by the beeswarm visualizations. Feature impact magnitudes and directions are mapped across the dataset. Through this approach, both feature importance and interactive effects are revealed [53]. The ranking of these input variables, reflecting their respective levels of importance, is presented in Figure 7. Figure 7(a) reveals that the RT has the highest mean SHAP value (0.58), indicating it plays a dominant role in model predictions. This is followed by CL and MTOR, both of which also show significant contributions. Figure 7(b) provides further insights into the distribution of each feature’s influence. Notably, higher reaction temperatures consistently increase the model output, aligning with known kinetic benefits in

biodiesel synthesis, which show that increased temperature lowers oil viscosity, leading to improved biodiesel yields [75]. Interestingly, while higher Methanol to Oil ratios reduce the output, suggesting a saturation or inhibitory effect, Catalyst Loading exhibits a non-linear pattern, possibly indicating an optimal range for efficiency. Overall, these findings validate the model's alignment with experimental expectations and

highlight the critical parameters for process optimization.

Table 7. Optimized process variables

Variables	Value
RT (°C)	66.25
CL (wt%)	6.37
Rt (min)	104.61
MTOR	8.84
Predicted Optimum Yield (%)	81.90
Experimental Optimum yield (%)	82.3 ± 0.8

Table 8. Comparison of optimization result with literature

Catalyst source	Feedstock	Optimum conditions	Biodiesel yield (%)	Reference
Ti-supported ZnO/TiO ₂ heterogeneous catalyst	WCO and soybean oil	Catalyst loading 21.9 wt%, 55 °C, methanol:oil 8:1	94.3	[7]
Biochar and calcined eggshell	WCO	61.5 °C, 2 wt% catalyst, 2.3 h, methanol:oil: 14.2:1	89.4	[20]
bio-based bifunctional catalyst	Waste cooking oil	60 °C, catalyst 5 wt%, 149.94 min, methanol:oil 13.03:1	93.0	[25]
waste marble tiles + cow horn	WCO	74.86 °C, 5.12 wt% catalyst, 11.43:1 methanol:oil, 119.92 min	98	[31]
Moringa leaves	Soybean oil	65 °C, 6 wt% catalyst, 6:1 methanol:oil, 3 h	86.7	[90]
Coconut shell and periwinkle shell	Waste cooking oil and animal fat	66.3 °C, 6.37 wt% catalyst, 11.43:1, 104.6 min.	82.3	This study

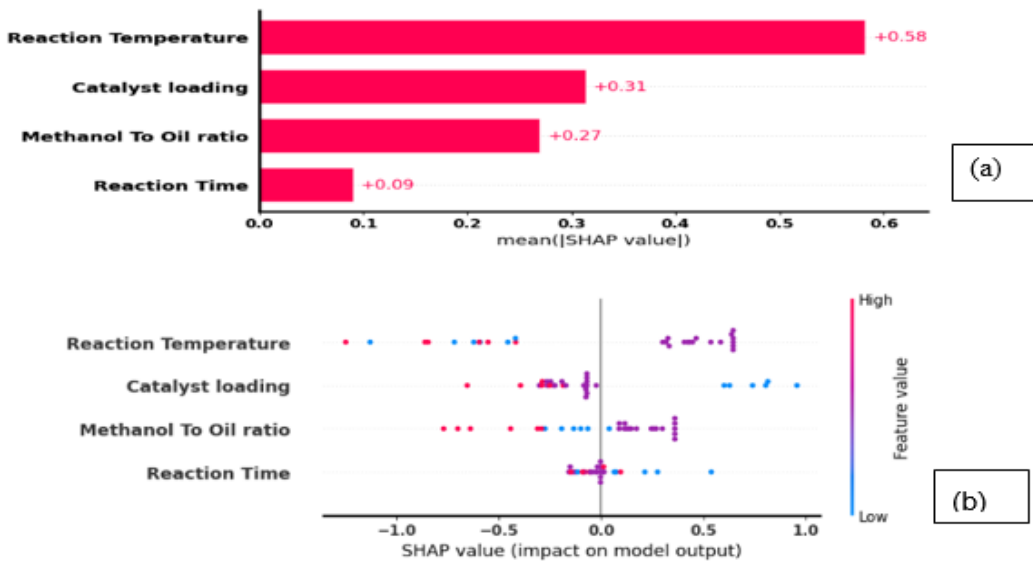


Figure 7. SHAP (a) feature ranking (b) beeswarm plot showing feature importance

3.6. Effect of catalyst reusability

Figure 8 illustrates the number of times the catalyst could be reused and the accompanying yield for each cycle. The catalyst exhibited remarkable stability, with the biodiesel yield decreasing only slightly from an initial 81.9% to 79.1% over five cycles. The total drop in yield was just 3.4% over the five-cycle period. This high retention of catalytic

activity (97.1% relative to the fresh catalyst) suggests that the active sites remained largely intact. This was achieved despite repeated recovery and washing steps using methanol and n-hexane. The sustained activity of the catalyst could be ascribed to the combined effect of the carbon support and the doped sites. The use of CS-BC provides a high surface area that holds the CaO particles derived from the periwinkle shells.

Mahmood and Al-Yaqoobi [82] demonstrated that waste-derived CaO systems (such as those from mango leaves) can maintain yields above 80% through five cycles when the active phase is properly stabilized. In this study, the CS-BC matrix likely limits the sintering of CaO particles. The incorporation of copper as a dopant enhanced the structural integrity of the catalyst. Comparable results were observed by Uzuegbu et al. [43] regarding periwinkle shell-based catalysts, where optimized shell-derived frameworks provided stable yields (up to 87%) in transesterification. The minor reduction in yield is likely due to active site masking. As noted by Aisien et al. [44] in their development of periwinkle shell catalysts, trace amounts of glycerol can physically block the catalyst pores over multiple runs, while minor leaching of calcium ions into the liquid phase might contribute to the observed slight decrease in activity [20, 23, 83]. This high reusability improves the potential for large-scale application because the catalyst does not need to be replaced frequently. In practical terms, this can reduce operating costs, lower the amount of catalyst required, and minimize waste generation during biodiesel production.

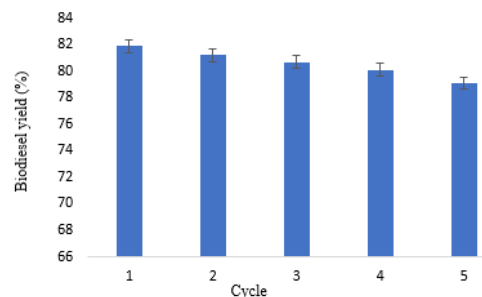


Figure 8. Catalyst recyclability

3.7 Physiochemical characteristics of the biodiesel
The fuel characteristics of the WCO-AF blend biodiesel synthesized using the CS-BC/CPS composite bifunctional catalyst are presented in Table 9, alongside relevant international standard specifications for comparative assessment. The acid value (0.45 mg KOH/g) and free fatty acid content (0.225%) are both below the EN 14104 limit of 0.5 mg KOH/g, indicating effective conversion and minimal corrosive potential. A density of 873 kg/m³ aligns with EN ISO 12185 specifications (860–900 kg/m³), supporting good fuel atomization. The flash point of 162°C exceeds the ASTM D6751 minimum of 93°C, confirming the absence of residual methanol and ensuring safe handling. The viscosity at 40°C (3.98 mPa·s) aligns with the EN 14214 acceptable range (3.5–5.0 mm²/s), suggesting proper flow and combustion characteristics. Additionally, the peroxide value of 0.69 meq/kg reflects excellent oxidative stability, well below commonly cited thresholds (≤ 5 meq/kg), indicating low degradation and good shelf life. These results collectively confirm that the biodiesel is of good quality,

Table 9. Physiochemical and fuel properties

S/N	Properties	Biodiesel	ASTM 6751 standards	EN14214 standard
1.	Acid Value (mg KOH/g)	0.45	0.8 max	0.5 max
2.	Free fatty Acid (%)	0.225	0.4 max	0.25 max
3.	Density at 25 °C (kg/m ³)	873	-	860–900
4.	Flash point (°C)	162.0	100 – 170	120 min.
5.	Viscosity @ 40 °C (mpas).	3.98	1.9–6.0	3.5–5.0
6.	Peroxide value (meq/kg)	0.69	-	-

4. Conclusion

This work successfully synthesized an innovative bifunctional catalyst derived from carbonized coconut shell and calcined periwinkle shell doped with copper nitrate. This sustainable catalyst demonstrated effective catalytic performance in the conversion of oil-fat blend into biodiesel. Biodiesel yield from this feedstock was further modeled using four machine learning algorithms, among which the Extreme Gradient Boosting model outperformed others in predicting biodiesel yield, with a high R^2 (0.899) and a low RMSE (0.230). The MRFO employed to enhance

transesterification efficiency established 66.3°C, 6.37 wt% catalyst, 104.6 minutes, and 8.84:1 MTOR as the optimum conditions. Furthermore, SHAP analysis revealed that reaction temperature had the greatest impact on biodiesel yield, followed by CL, MTOR, and Rt. This finding offers significant understanding regarding process dynamics and parameter prioritization. The catalyst performed consistently well over multiple cycles. Retaining more than 97% of its initial activity after five cycles indicates good durability. From a practical perspective, this level of stability makes it a promising alternative to homogeneous catalysts,

especially in the context of waste-to-energy systems where cost, reuse, and scalability are key considerations. Characterization of the synthesized biodiesel revealed that all major fuel properties were within the limits specified by international standards (ASTM D6751 and EN 14214), confirming the high quality and suitability of the biodiesel for engine utilization.

In the optimization study, certain limitations may have constrained further yield enhancement. The low epoch and population settings, while computationally efficient, might have curtailed the

algorithm's exploration capabilities. Future studies can benefit from exploring larger population sizes, increased epoch counts, and hybrid MRFO methods that incorporate local search techniques. Also, adopting multi-objective MRFO could enhance practical relevance by balancing yield while minimizing reaction time or energy consumption. Additionally, future work should explore real-engine performance testing to further establish the industrial applicability of this integrated approach.

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