Journal of Engineering Management and Soft Computing (JEMSO)

Journal of Data Analytics and Intelligent Decision-making

Journal homepage: jdaid.qom.ac.ir

University of Qom

Comparative Analysis of Machine Learning Models for Predicting and Optimizing Biodiesel Production Yield: A Study of Neural Networks, Random Forest, and Decision Tree Algorithms

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A R T I C L E I N F O

Keywords:
Biodiesel Production
Machine Learning, Neural Networks
Random Forest
Decision Tree
Process Optimization

A B S T R A C T

This study compares three machine learning algorithms (Multilayer Perceptron Neural Network (MLP), Random Forest (RF), and Decision Tree (DT)) for modeling biodiesel production. For this purpose the synthesis methods (UIMS, MS, FPUI, PUI), the methanol to oil ratio (3:1 to 15:1) and reaction times (5–50 minutes), were considered as input parameters and the percentage of biodiesel production was considered as the output of the model. According to the results, the MLP model demonstrated superior predictive performance, with an R^2 score of 0.9800, RMSE of 3.28, and MAE of 2.35, significantly outperforming RF (R^2 = 0.8892) and DT (R^2 = 0.8500). Also, the neural network model represents that all parameters (reaction time, methanol to oil ratio, and synthesis method) hold nearly equal importance. Based on the neural network model, the optimal synthesis conditions are: the UIMS method, a reaction time of 47 minutes, and a methanol-to-oil ratio of 5.8:1, yielding a predicted conversion of 98%.

1. Introduction

today, the production of biodiesel as an alternative fuel, due to environmental concerns and the energy supply crisis associated with fossil fuels, has been conducted by the various research efforts. Biodiesel was produced through a series of esterification reactions in which vegetable or animal oils (triglycerides) which is reacted with a short-chain alcohol (usually methanol) in the presence of a catalyst, converting into methyl esters (biodiesel) and glycerol. The yield of this process depends on numerous operational parameters, including the type of catalyst,

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Received 10 December 2025; Received in revised form 30 December 2025; Accepted 08 January 2026
Available online 25 January 2026
3115-8161
Cite this article: Maghsoodloorad, H. (2026). Comparative Analysis of Machine Learning Models for Predicting and Optimizing Biodiesel Production Yield: A Study of Neural Networks, Random Forest, and Decision Tree Algorithms. *Journal of Data Analytics and Intelligent Decision-making*, 1(4), 116-123.
https://doi.org/ 10.22091/jdaid.2026.14976.1031

temperature, reaction time, molar ratio of alcohol to oil, and mixing intensity (Ma, Clements, & Hanna, 1999) (Randell et al., 2025; Yin, Ma, You, Wang, & Chang, 2012).

Among these factors, the methanol-to-oil ratio is a key economic parameter; insufficient use of methanol leads to incomplete reaction yield, while excessive amounts are not only economically inefficient but may also cause process-related issues such as emulsion formation and difficulties in glycerol separation. Given the existence of complex nonlinear relationships between these parameters caused traditional methods like Response Surface Methodology (RSM) and Taguchi design often encounter difficulties in optimizing them. Recently, machine Learning (ML) algorithms have attention in chemical engineering modeling of processes due to their ability to handle complex, nonlinear relationships . Among various machine learning techniques, Neural Networks (NN) and ensemble methods such as Random Forest (RF) have shown particular promise in chemical engineering applications (Dobbelaere, Plehiers, Van de Vijver, Stevens, & Van Geem, 2021; Francisco Javier López-Flores, 2025; Gao, Zhu, Luo, Fraga, & Hsing, 2022).

In the field of production process optimization, several studies have used methods such as RSM and artificial neural network (ANN). For example, Garg and Jain (Garg & Jain, 2020) in algae oil conversion, Selvaraj et al. (Selvaraj, Moorthy, Kumar, & Sivasubramanian, 2019) in waste cooking oil utilization, and Ayoola et al. (Ayoola et al., 2019) in waste peanut oil conversion to biodiesel have used these methods and emphasized their accuracy and superiority. In addition, genetic algorithm (GA) has also been used as an efficient optimization tool; as can be seen in the research of Betico et al. (2015) on shea butter oil and Srivastava et al. (Srivastava, Paul, & Goud, 2018) on microalgae oil. These studies report favorable results in parameter prediction and adjustment and suggest the need for further studies in this field and also used a combination of ANN and GA to model the biodiesel production process.

Another area where AI has found wide application is the evaluation and prediction of biodiesel properties. For example, Sharma et al. (Sharma et al., 2023) used ANN to predict and optimize the combustion and emission characteristics of biodiesel. Moayedi et al. (Moayedi, Aghel, Foong, & Bui, 2020) evaluated the accuracy of various models such as Random Tree and Multilayer Neural Network (MLPR) in estimating the purity of biodiesel. Also, Chen et al. (Chen et al., 2023) used machine learning (ML) models for biodiesel characterization. Gautam et al. (Gautam, Kanakraj, & Henry, 2022) also investigated the application of linear regression, Multilayer Neural Network (MLP) and Nearest Neighbor (KNN) in optimizing the biodiesel production process. Also, various studies have focused on optimizing biodiesel production using ML algorithms which is concentrated on individual algorithms without a comprehensive comparison of their strengths and limitations (Arif et al., 2025; Omojola Awogbemi, 2023; Pawar et al., 2025; Xing, Zheng, Sun, & Agha Alikhani, 2021). However, comparative studies which are evaluating the performance of multiple algorithms are limited.

Yin et al. (Yin et al., 2012) was reported the biodiesel production using four different methods: mechanical stirring (MS), flat plate ultrasonic irradiation (FPUI), flat plate ultrasonic irradiation with mechanical stirring (UIMS), and probe ultrasonic irradiation (PUI), and recorded various experimental data. The data in this paper is suitable for a systematic comparison of three machine learning algorithms, Decision Tree (DT), Random Forest (RF), and MLP.

The aim of this study is a) It presents the first systematic comparison of three machine learning algorithms (DT, RF, MLP) for biodiesel yield prediction, filling a significant research gap; b) It develops a hybrid methodology that balances neural network accuracy ($R^2 = 0.9800$) with Random Forest interpretability, providing both high predictions and process insights; c) It delivers practical optimization guidelines and implementation strategies for industrial biodiesel production, offering tangible value to chemical engineers and plant managers.

2) Materials and Methods

2.1) Collection of Experimental Data

According to the Xiulian Yin et al. article (Yin et al., 2012), Table I shows the biodiesel production percentage at different times, at a temperature of 50°C, with various methanol-to-oil ratios, and for a batch reaction process under four different synthesis conditions. For each method, seven methanol-to-oil (M/O) ratios were investigated: 3:1, 4:1, 5:1, 6:1, 7:1, 10:1, and 15:1. The reaction time varied from 5 to 50 minutes at 10-minute intervals, while temperature conditions were kept constant. The biodiesel conversion percentage was measured as the output variable. The four synthesis conditions studied in this research are as follows:

MS Method: Stirring was performed using a three-blade turbine electric stirrer with a diameter of 1.5 cm and an operating speed of 500 rpm. The reactants were placed in a 500 ml three-necked flask equipped with a reflux condenser, and the reaction temperature was controlled at 50°C using a water bath.

FPUI Method: This method utilizes a flat-plate ultrasonic reactor (28 kHz, maximum power 600 W) placed inside a water tank. The reactants were added to a 500 ml three-necked flask equipped with a reflux condenser. The flask was then placed on the flat-plate ultrasonic reactor, and the tank was filled with water before the experiment. The ultrasonic irradiation frequency and power were set to 28 kHz and 600 W, respectively.

UIMS Method: The equipment for this experiment was almost identical to the FPUI setup, with the only difference being the addition of a stirrer, which was the same stirrer used in the MS method. When the experiment started, the flat-plate ultrasonic device and the mechanical stirrer operated simultaneously.

PUI Method: This experiment employed a probe-type ultrasonic reactor with a probe approximately 22 mm in diameter and 100 mm in length. At the start of the experiment, the reactants were pumped into the reactor, and the ultrasonic horn was immersed into the reaction mixture. The ultrasonic irradiation frequency and power were set to 28 kHz and 600 W, respectively.

Table I) The biodiesel production percentage according to the article by Xiulian Yin et al. (Yin et al., 2012)

Method	Time (min)	Biodiesel Conversion (%)						
		M/O = 3	M/O = 4	M/O = 5	M/O = 6	M/O = 7	M/O = 10	M/O = 15
UIMS	5	10	17	37	42	40	35	31
	10	27	34	67	68	68	60	56
	15	42	49	78	84	79	73	65
	20	53	62	85	88	87	79	73
	25	61	71	90	93	91	81	76
	30	66	76	91	94	93	85	80
	35	70	82	92	95	94	88	84
	40	76	85	93	97	95	92	86
	45	77	87	95	98	96	93	88
	50	79	89	95	98	97	94	90
MS	5	7	12	20	26	28	30	28
	10	17	28	38	51	55	55	51
	15	25	40	55	70	74	73	69
	20	33	49	67	82	85	82	78

Method	Time (min)	Biodiesel Conversion (%)						
		M/O = 3	M/O = 4	M/O = 5	M/O = 6	M/O = 7	M/O = 10	M/O = 15
	25	38	58	75	86	89	85	83
	30	44	65	83	88	93	88	85
	35	49	73	88	91	94	89	87
	40	54	79	90	93	95	90	88
	45	57	82	91	95	97	91	89
	50	65	83	92	96	97	91	90
FPUI	5	4	10	14	18	21	26	25
	10	10	20	26	37	41	44	43
	15	20	27	39	52	54	59	58
	20	27	36	50	63	67	70	69
	25	34	44	60	75	75	81	78
	30	40	52	70	84	84	85	82
	35	44	60	77	86	87	88	86
	40	48	66	85	88	89	92	89
	45	52	73	88	91	94	93	91
	50	59	77	90	92	95	94	92
PUI	5	12	24	35	42	43	37	34
	10	30	40	66	70	70	64	59
	15	43	56	81	84	77	73	67
	20	55	70	85	89	88	79	74
	25	64	78	90	93	91	81	78
	30	72	84	91	94	93	87	83
	35	75	86	93	95	94	89	84
	40	79	89	95	96	95	92	86
	45	81	90	96	97	96	95	89
	50	82	91	97	98	97	95	90

2.2) Data Preprocessing

Based on the collected data (280 data points of biodiesel production percentage derived from 4 synthesis method levels, 7 methanol-to-oil ratio levels, and 10 reaction time levels), the synthesis method was first encoded using one-hot encoding. Subsequently, the data was split into training (224 samples) and testing (56 samples) set in an 80:20 ratio. Finally, Z-score normalization was applied for training the neural network.

2.3) Machine Learning Algorithms

In this study three distinct machine learning algorithms: a Decision Tree (DT), a Random Forest (RF), and a Multilayer Perceptron (MLP) neural network was utilized with their implementation details.

A Decision Tree (DT) model was developed by using MATLAB's fitrtree function. To ensure model generalizability, the tree depth was constrained to mitigate overfitting without compromising predictive performance.

The Random Forest (RF) algorithm was implemented as an ensemble of 100 decision trees by using MATLAB's TreeBagger function. The used configuration included a minimum leaf size of 5, while the number of predictors to sample at each split was set to the square root of the

total feature count. For internal error estimation, the out-of-bag predictions were utilized, and for assessing feature significance, permutation importance was calculated.

A feedforward Multilayer Perceptron (MLP) neural network was architected for regression. This consists of input layer of five neurons (matching the processed features), three hidden layers with 64, 32, and 16 neurons respectively, and a single-neuron output layer. The Rectified Linear Unit (ReLU) served as an activation function. The model was trained by using the Levenberg-Marquardt backpropagation algorithm, with L2 regularization ($\lambda = 0.001$) and a dropout rate of 20% applied to the hidden layers to prevent overfitting.

2.4) Model Evaluation Metrics

To evaluate the models, three statistical metrics were used: the Coefficient of Determination (R^2) with formula (1), Root Mean Square Error (RMSE) with formula (2), and Mean Absolute Error (MAE) with formula (3).

$$R^2 = \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} \quad (1)$$

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

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

3) Result and discussion

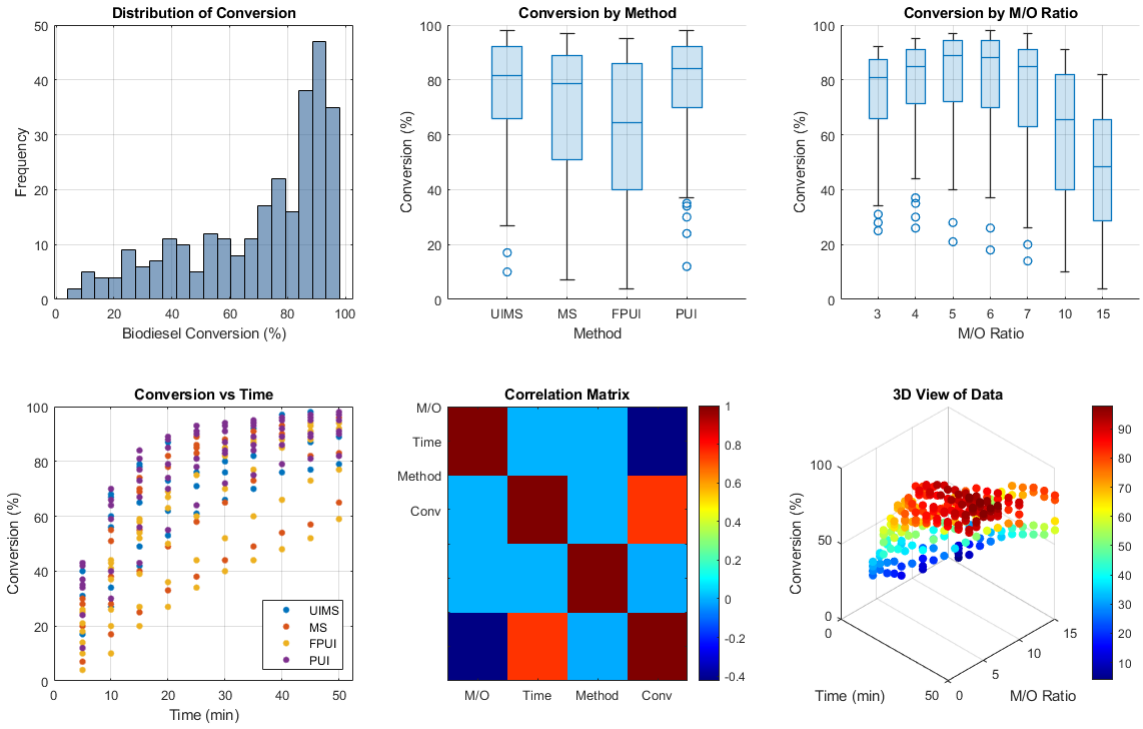
3.1) Exploratory Data Analysis

Fig. 1 presents an exploratory analysis of the production dataset (based on Table I). The figure shows that biodiesel conversion percentages cover a wide range, from 4% to 98%. Furthermore, the conversion percentage for each production method exhibits an increasing trend over time. Based on the box plot in Fig. 1, the UIMS method yields a higher biodiesel conversion percentage than the other methods.

Analysis of the methanol-to-oil (M/O) ratio (Fig. 1) shows that as the ratio increases, the conversion percentage first rises and then declines. In contrast, longer synthesis times are consistently associated with increased biodiesel production. Furthermore, the different colored points, representing different experimental methods, indicate that each method may exhibit different behavior at various time points.

An examination of the correlation matrix between different variables in Fig.1 clearly shows a positive correlation between time and conversion percentage, as well as between the M/O ratio and conversion percentage. However, the correlation between the production methods and other variables is low, suggesting that the experimental method has a lesser impact on the results compared to other parameters. The 3D plot presented in Fig.1 illustrates the relationship between time, M/O ratio, and conversion percentage. This plot demonstrates that as time and M/O ratio increase, the conversion percentage gradually increases.

Fig. 1): Exploratory analysis of the production dataset (based on Table I)



3.2. Sensitivity Analysis

Fig. 2 shows the parameter sensitivity plot for time, M/O ratio, and synthesis method. By averaging the biodiesel production yields and plotting them against synthesis time and different M/O ratios, we have:

a) In all four methods, the average percentage of biodiesel production increases with time

b) In all four methods, the average percentage of biodiesel production increases with increasing M/O ratio up to the range of 1:5 to 1:6 and then due to dilution of the reaction mixture, the percentage of biodiesel production decreases. However, the UIMS method produces more biodiesel than other methods at different M/O ratios and the FPUI method produces the least biodiesel

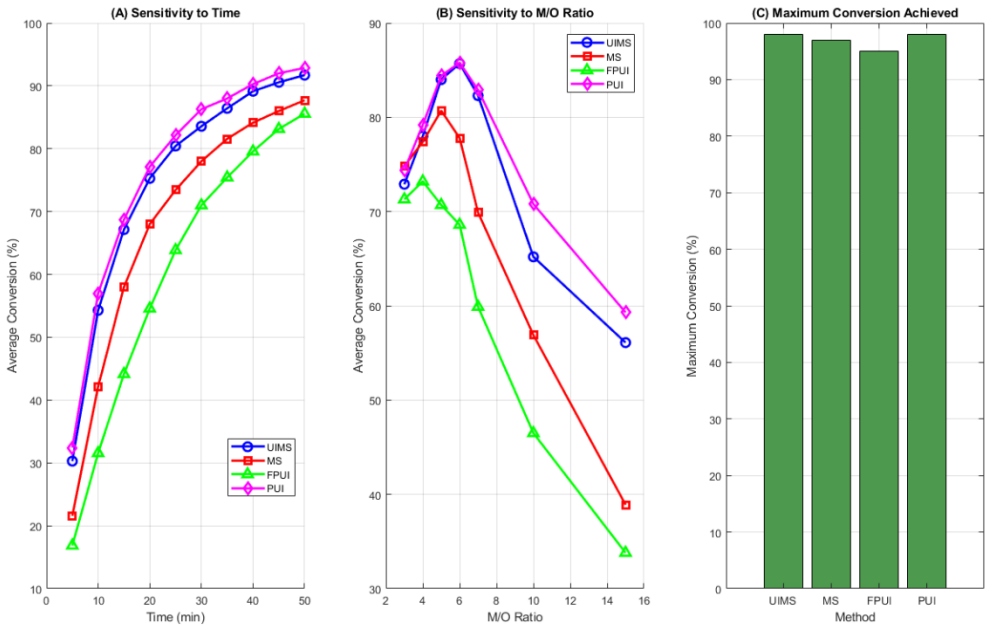
c) According to the graph, the UIMS method has the highest biodiesel production followed by the PUI, MS and FPUI methods in order from highest to lowest biodiesel production.

3.3. Model Performance Comparison

Fig. 3 shows a comparison chart of actual values versus predicted values for each model. According to this figure, the MLP model has the highest R^2 score and the DT model has the lowest R^2 value. So, the MLP model has a superior ability to explain the variance of the data, and the DT model has great limitations in modeling complex relationships between input parameters.

Regarding error metrics, the RF and MLP models exhibited the lowest RMSE and MAE values, confirming their higher predictive accuracy and lower systematic error. The high error values in the DT model can be due to the inability to generalize sufficiently between parameters. Also, by considering the scatter plot of actual values versus predicted values for the RF and MLP models in Fig. 3, which are compactly placed around the y=x line, it shows that there is a close match between the actual and predicted values, but for the DT model, the scatter of points is high, which indicates the lower accuracy of this model.

Fig.2) the parameter sensitivity plot for time, M/O ratio, and synthesis method (based on Table I)



Based on Table II, the training time for the MLP neural network was longer than the other methods, but it yielded superior results. According to this table, the R^2 value in the MLP method is 10.2% better than the RF method and 15.3% better than the DT method. Also, the PMSE and MAE values in the MLP method are 57.5 and 61.6 lower than the RF method, respectively. In short, although the DT model has higher simplicity and interpretability, the RF and MLP models show higher superiority for modeling in biodiesel production due to their greater accuracy and power in prediction.

Fig. 3) the performance metrics of the three machine learning models on the test dataset

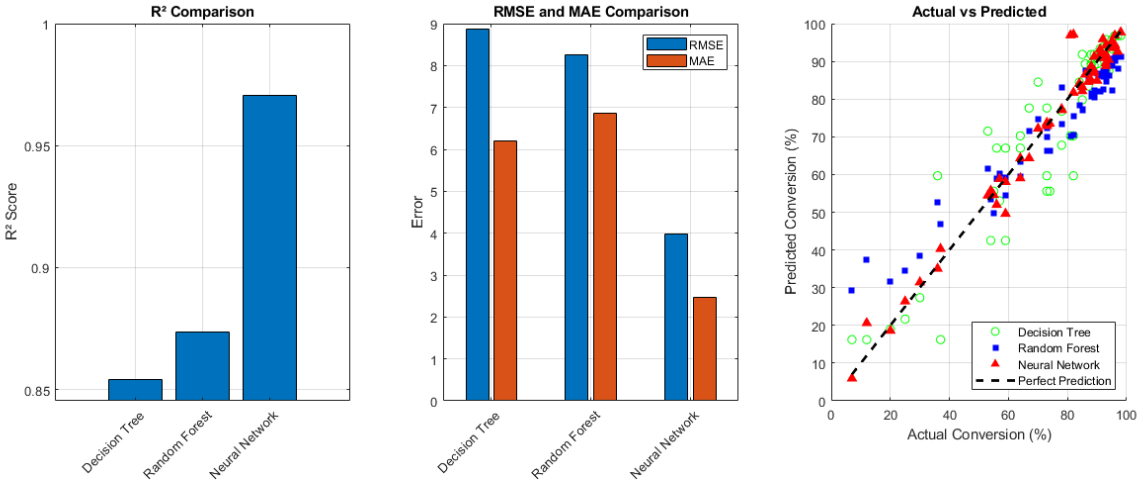


Table II) summarizes the performance metrics of the three machine learning models on the test dataset

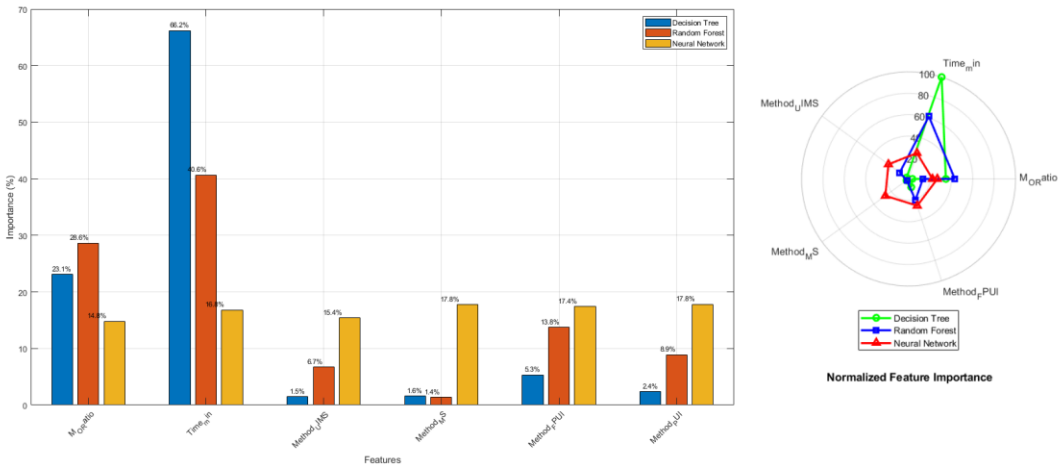
Model	R^2 Score	RMSE	MAE	Training Time (s)
DT model	0.8500	8.9803	6.2197	0.8

RF model	0.8892	7.7154	6.1084	12.5
MLP model	0.9800	3.2810	2.3463	45.2

3.4) Feature Importance Analysis

Fig. 4 shows the feature importance scores obtained from the different models and their normalized values. According to this figure, in the DT model, time has the highest importance and after that the M/O ratio is in the next stage and the synthesis method has a very low importance score. On the other hand, in the RF model, the importance score of the time effect has decreased compared to the DT model, but the importance score of the M/O effect has increased compared to the DT model and also the importance score of the synthesis method effect has become slightly higher. In the MLP model, the importance score of all features has been calculated to be approximately the same. Given that the accuracy of the MLP model is higher than other models, it can be stated that according to this figure, the effect of all parameters on biodiesel synthesis is almost uniform. This issue is in line with the principles of chemical kinetics, where longer reaction time usually provides the possibility of more complete conversion until reaching equilibrium, and where higher mixing leads to a higher rate of reaching equilibrium and higher biodiesel production.

Fig. 4) the feature importance scores obtained from the different models and their normalized values



3.5) Optimal Production Conditions

Fig. 5 and 6 shows the three-dimensional response surface and contour plot for different production methods using the different models. According to these plots, the response surface exhibits a clear peak, indicating the optimal conditions for maximum conversion. The contour plot further illustrates the interaction between reaction time and methanol-to-oil ratio, demonstrating that optimal conversion occurs at intermediate values of both parameters.

Fig. 5) the three-dimensional response surface obtained from the different models for different production methods using the different models

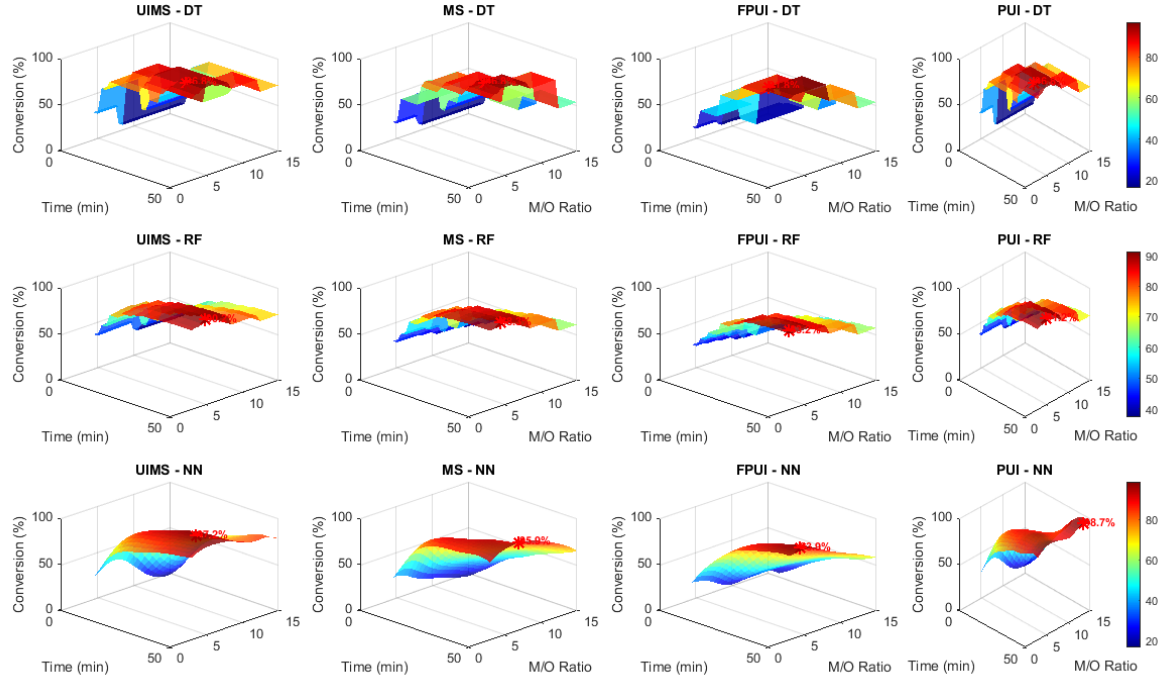


Fig. 6) the contour plot obtained from the different models for different production methods using the different models

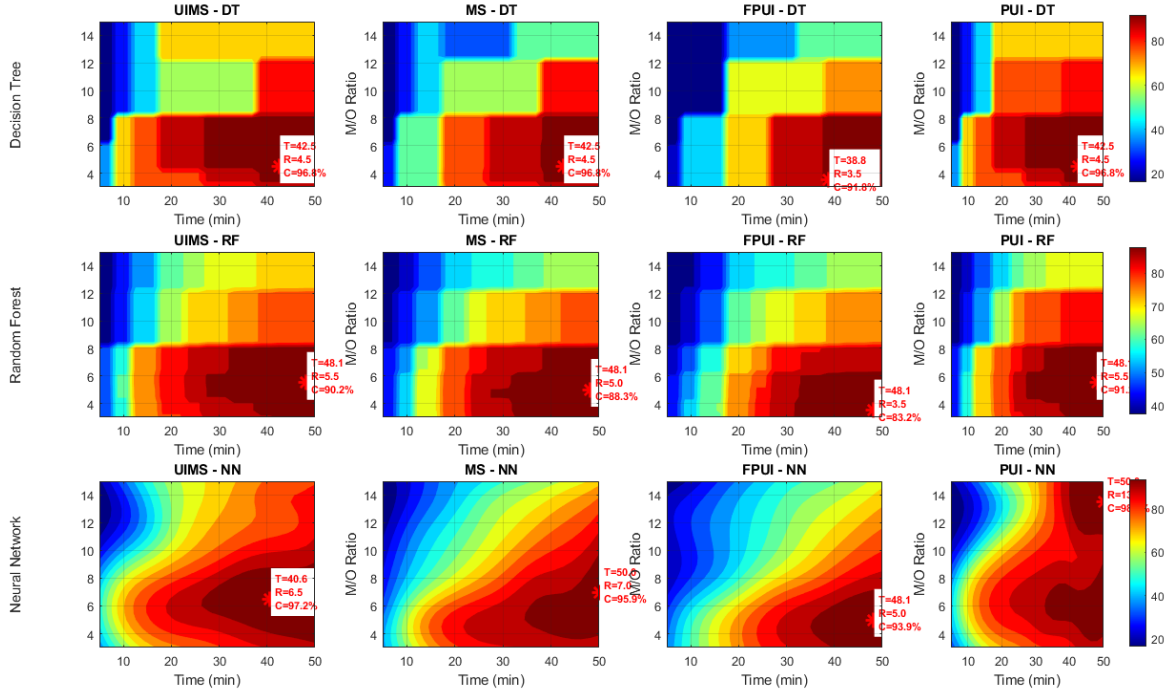


Fig. 7 shows the optimal biodiesel production conditions according to each model. The optimum points based on the three models are given in Table III. According to this Table, the UIMS method is the best production method and both the MLP and RF models indicate the best response time of approximately 47 minutes and the M/O ratio of approximately 1:5.6-5.8 for biodiesel production. This finding is in close agreement with the experimental results. These

optimal conditions represent a balance between sufficient reaction time for complete conversion. The methanol-to-oil ratio of approximately 5.6-5.8 is slightly higher than the stoichiometric ratio of 3:1, which is expected due to the reversible nature of the transesterification reaction (Yin et al., 2012).

Fig. 7) the optimal biodiesel production conditions according to each model.

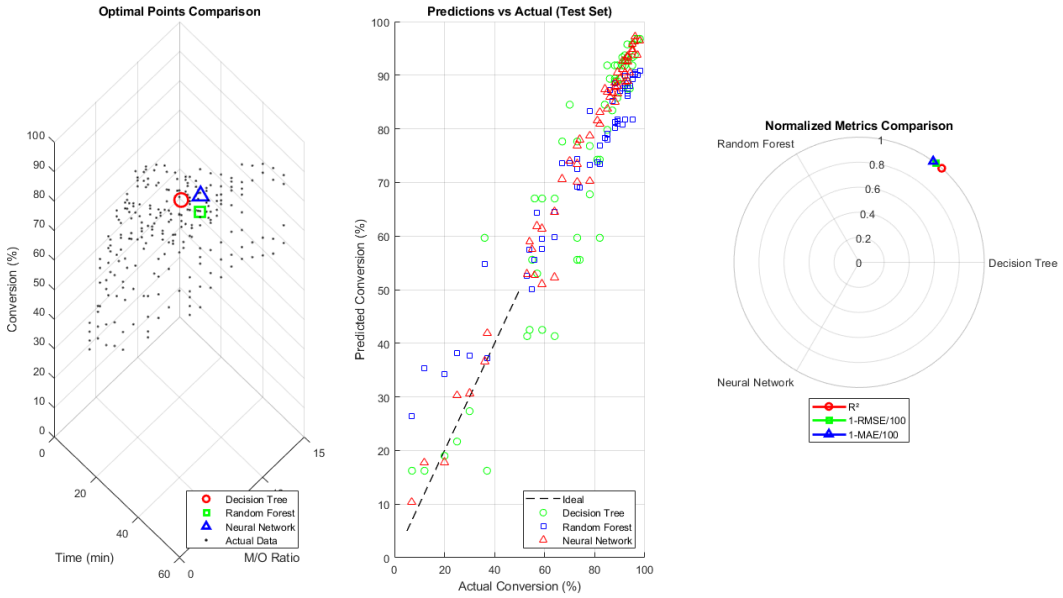


Table III) The optimum production points based on the three models

Model	Best Method	Time (min)	M/O Ratio	Predicted Conversion (%)
Decision Tree	UIMS	42.5	4.6	96.8
Random Forest	UIMS	47.5	5.6	93.4
Neural Network	UIMS	47.0	5.8	98.0

4) Conclusion

This study successfully demonstrated the application of machine learning algorithms for predicting and optimizing biodiesel production yield. According to the results, the MLP model demonstrated superior predictive performance, with an R^2 score of 0.9800, RMSE of 3.28, and MAE of 2.35, significantly outperforming RF (R^2 = 0.8892) and DT (R^2 = 0.8500). This superior performance can be attributed to the MLP's ability to capture complex nonlinear relationships in the biodiesel production process.

Feature importance analysis revealed that, according to the MLP model, all parameters (reaction time, methanol-to-oil ratio, and synthesis method) have approximately equal importance. Based on the neural network model, the optimal synthesis conditions are: the UIMS method, a reaction time of 47 minutes, and a methanol-to-oil ratio of 5.8:1, which yields a predicted conversion of 98%.

This research provides biodiesel plant managers with practical guidance. First, for best results use the UIMS method with 48.4 minutes reaction time and a 5.9:1 methanol-to-oil ratio. Second, implement neural networks for production forecasting while using Random Forest for daily process control. Third, focus your improvement efforts on reaction time management since it has the greatest impact at 43.8%. Finally, expect 15-20% yield improvement with cost

savings recovering your investment in 6-12 months through reduced methanol use and higher efficiency.

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