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Application of Machine Learning for Methanolysis of Waste Cooking Oil Using Kaolinite Geopolymer Heterogeneous Catalyst

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INTRODUCTION

Biodiesel, a promising biofuel derived from vegetable oils or animal fats, offers a sustainable alternative to conventional fossil fuels. The Methanolysis process, a key step in biodiesel production, traditionally employs homogeneous catalysts (acids or bases)(Mwenge et Seodigeng). However, these catalysts pose challenges due to separation difficulties and potential contamination of the final product. Recent research explores geopolymers as heterogeneous catalysts, addressing these limitations.

Geopolymers are inorganic polymers synthesised from readily available aluminosilicate sources like metakaolin using alkaline solutions. Their porous structure makes them ideal candidates for heterogeneous catalysis in biodiesel production. They are reusable and environmentally friendly, contributing to the green biodiesel process (Boti et al, 2020).

Machine learning (ML) offers a powerful approach and revolutionising biodiesel production by enabling predictive modeling and process optimisation (Gupta et al, 2021).

This report explores the use of geopolymer heterogeneous catalysts and machine learning (ML) for a more sustainable and efficient biodiesel production process. Three machine learning algorithms, response surface methodology (RSM), artificial neural network (ANN), and adaptive neuro-fuzzy inference system (ANFIS), were used to optimise and model biodiesel production from waste cooking oil catalysed by kaolinite geopolymer using process parameters, such as methanol-to-oil ratio, catalyst loading, reaction temperature, and reaction time.

METHOD

Kaolinite geopolymer was prepared by reacting activation with metakaolin; metakaolin was prepared by calcining kaolin heavy pure as a source of aluminosilicate. The activation solution was prepared by mixing a 12M NaOH solution with a 1.5SG activation solution. The geopolymer was left to cure for 5 days at room temperature. The geopolymer was prepared with the targeted molar ratio of SiO2/Al2O3 = 4.0, SiO2/Na2O = 3.1, and H2O/Na2O = 14.2 for the Na-GP system and SiO2/Al2O3 = 4.0, SiO2/K2O = 3.1 and H2O/K2O = 14.2 for the K-GP system. (Botti et al., 2020).

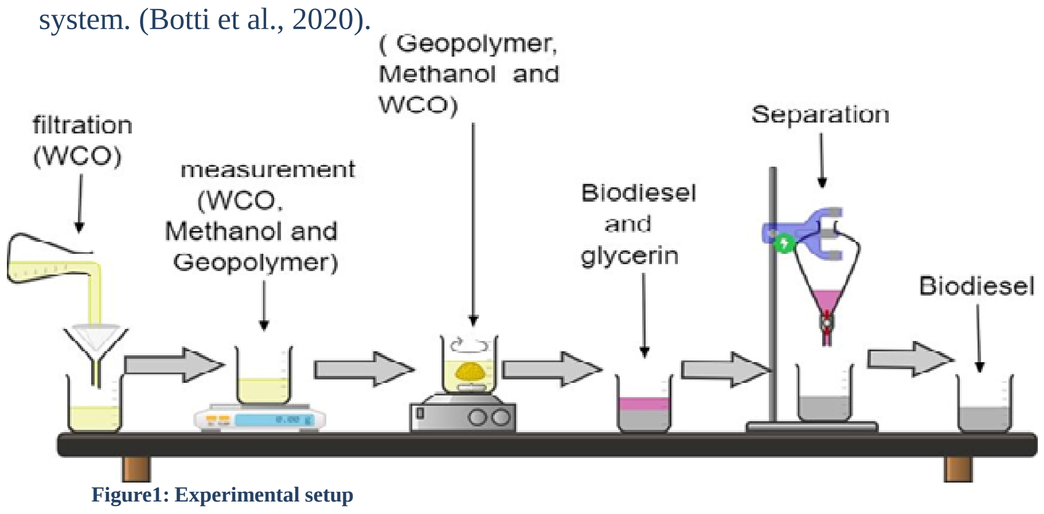


Figure1: Experimental setup

Table 1: Range of process parameters used for the models

Input	Range	Output
Methanol/Oil ratio (wt. %)	10-20	Yield (%)
Catalyst ratio (wt. %)	2-6	
Time (h)	2-6	
Temperature (°C)	60 -120	

The produced geopolymer was used to produce biodiesel using conditions as in Table 1. The description of the methanolysis is described in Figure 1. Once the biodiesel was produced, it was separated using a separating funnel for 4hrs. Biodiesel yield was calculated using Equation (1)

$$\text{Biodiesel yield} = \frac{Mass\ of\ biodiesel}{Mass\ of\ Oil} \quad (1)$$

RESULTS & DISCUSSION

RSM was applied in Design Expert 13, and Neural Network Modular and Neuro-fuzzy were built with an NN toolbox using MATLAB 2021. 26 experimental data were randomly divided into 70 % for training and 30% for validation and testing. The ANN architecture is shown in Figure 2.

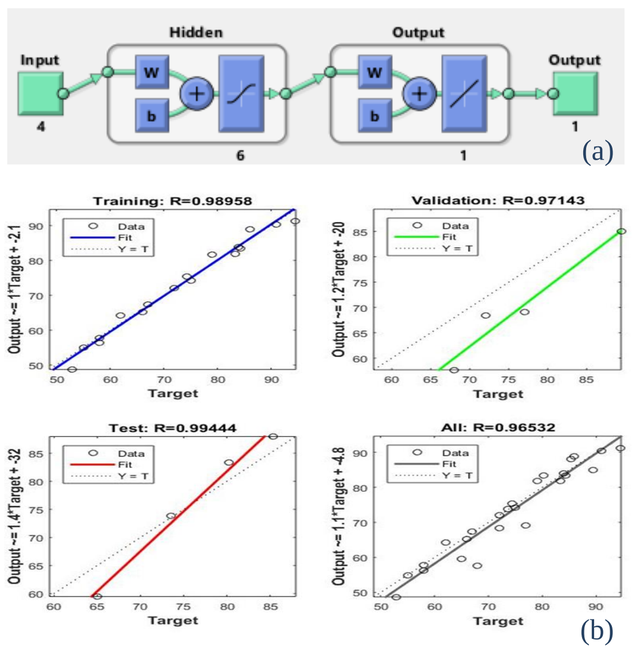


Figure 2. (a)The architecture of the ANN model. (b)Training, validation, and testing for the Levenberg-Marquardt algorithm.

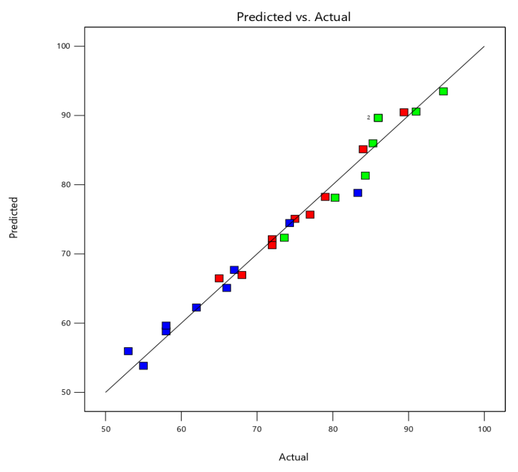
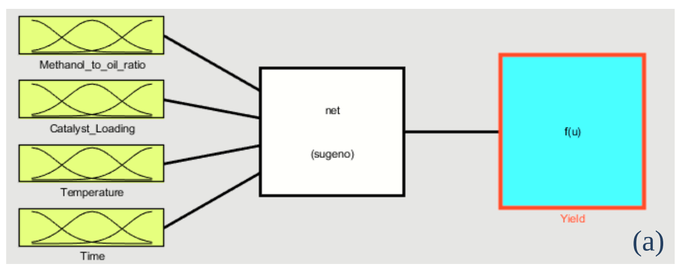


Figure 3. (a)Experimental vs Predicted data from RSM

Numeral optimisation was performed in RSM, and the results obtained show optimum conditions at 15 wt.% of methanol/oil, 4 wt.% catalyst, 4h and 120 reaction temperature.

Figure 3 depicts how the network interacts with the training, testing, and validation data. The correlation coefficients for the training, testing, validation, and test data were found to be 0.990, 0.994, 0.971, and 0.965, respectively. The straight line also demonstrates the linear connection.



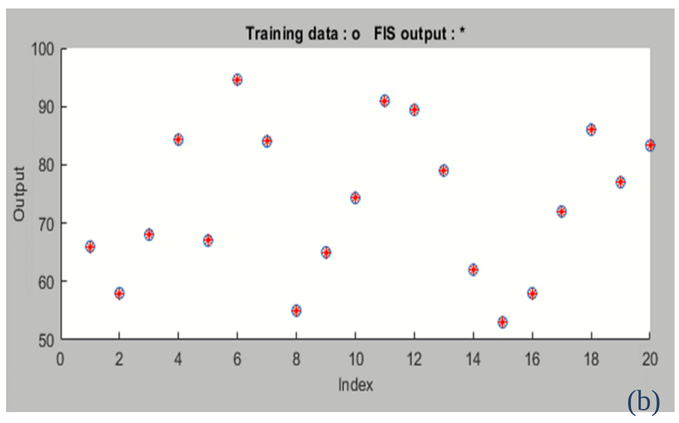


Figure 4. (a) The architecture of the ANFIS model.
(b) Actual and Predicted Adsorption Data for ANFIS.

Table 2: Error metrics used to evaluate the models

Error metrics	RSM	ANN	ANFIS
R^2	97.45	0.96532	0.9695
MSE	3.36049	5.03786	4.5739
RMSE	1.83316	2.24452	2.13867
MAE	1.41385	1.76933	0.74752
MAPE	1.90697	2.3644	0.94813
ARE	0.01907	0.02364	0.00948
MPSD	12.0864	15.1254	6.39025

From the error metrics which were used to evaluate the effectiveness of the models, ANFIS has the best performance as shown in Table; this is because ANFIS used the advantage of Neural network and Fuzzy logic. ANFIS has the benefit of being able to handle both numerical and language input variables in adsorption results analysis. This makes it effective for simulating systems where certain input variables are challenging to quantify or when data is ambiguous (Banza & Seodigeng)

CONCLUSION

The application of machine learning algorithms has improved the methanolysis process, leading to more efficient and predictable outcomes.
The use of kaolinite geopolymer as a heterogeneous catalyst is a sustainable and cost-effective alternative to traditional catalysts.
The findings suggest that integrating machine learning with chemical processes for biodiesel production can pave the way for more innovative and eco-friendly energy solutions.

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