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Modelling and Optimization of Bioethanol Production from Cassava Waste Slurry Using Artificial Neural Network and Adaptive Neuro-fuzzy Inference Systems

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Abstract

The increasing demand for alternative renewable energy sources has driven research into bioethanol production as a sustainable solution. This study investigates the production of bioethanol from cassava waste slurry using *Saccharomyces cerevisiae*. Process optimization and predictive modeling were conducted using Artificial Neural Networks (ANN) and Adaptive Neuro-Fuzzy Inference Systems (ANFIS). The research involved experimental fermentation, data collection, and computational modeling to analyze the effects of temperature, pH, and sugar concentration on ethanol yield. A total of 19 experimental runs were conducted, and the models were evaluated based on statistical indices, including mean square error (MSE) and coefficient of determination (R^2). The results demonstrated that ANFIS exhibited superior predictive accuracy, with an R^2 value of 0.9999 and a minimal error of 0.0000013607, outperforming ANN. The optimal conditions for bioethanol production were identified as 32.5 °C, 0.238 mol/dm³ sugar concentration, and pH 5.25, yielding 30% ethanol. Fourier Transform Infrared (FTIR) spectroscopy confirmed the presence of ethanol, validating the effectiveness of the fermentation process. The findings highlight the potential of cassava waste as a viable feedstock for sustainable bioethanol production and emphasize the advantage of soft computing techniques in optimizing bioethanol yield. These results contribute valuable insights into biofuel research, paving the way for efficient, cost-effective, and environmentally friendly bioethanol production processes.

Keywords: Artificial neural networks; adaptive neuro-fuzzy inference systems; bioethanol; coefficient of determination; mean square error

1. Introduction

The escalating global consumption of fossil fuels and the resultant greenhouse effects have given rise to environmental contamination and climate change concerns (Dhande *et al*., 2021; Cai *et al*., 2022). Bioenergy is receiving increased attention in the industrial sector as part of the energy transition. This is due to the widespread availability of raw materials used for its production and the environmentally friendly fuel produced through the bio-conversion of these abundant raw materials (Tropea *et al*., 2022). Bio-fuels such as bioethanol, biogas, biodiesel, and bio-hydrogen have become feasible alternatives to diminishing fossil fuel reserves (Falowo *et al*., 2022). Bioethanol is a highly common liquid biofuel globally, valued at $6.8 billion in 2019 and expected to increase to $7.2 billion by 2024 (An *et al*., 2021).

Biofuels, obtained from biomass by biological, thermal, or chemical methods, are regarded as significant sources of renewable energy that can promote the sustainable development of economies. One popular choice for alternative liquid fuel in transportation is bioethanol and its blends. It can be used alone or mixed with traditional fossil fuels or biodiesel. When blended with biodiesel, the resulting fuel has better combustion properties (Teoh *et al*., 2019). Bioethanol is produced via the process of sugar fermentation by a variety of yeasts and bacteria, ultimately leading to its production as the end product of metabolism. In recent years, numerous research projects have concentrated on enhancing the process of turning diverse waste and residual substances into ethanol for fuel by alcoholic fermentation. These studies were aimed at increasing the efficiency of bio-conversion, maximizing ethanol production, and achieving higher concentrations of ethanol (Sarris and Papanikolaou, 2016). In order to ensure the sustainable and large-scale production of bioethanol, it is imperative to utilize biomass varieties that are abundant, renewable, and incur minimal or no expenses. Ideally, these biomass should also require minimal pretreatment before they can be used.

Several researchers have investigated the production of bioethanol from different carbohydrate-based substrates and wastes, including domestic food wastes (DFWs). These studies have proposed various fermentation strategies, including the use of monocultures of bacteria or yeasts (Selim *et al*., 2020), as well as mixed cultures of yeasts, fungi, and bacteria (Farias and Maugeri Filho, 2019). Contrary to agricultural and forestry residues, such as pruning and olive mill wastes, as well as other forms of biomass that have been utilized for the production of bioethanol and other biofuels, dried food waste (DFW) does not require any intricate thermal, chemical, as well as thermochemical pretreatment procedures in order to be converted into biofuels by microorganisms (Farias and Maugeri Filho, 2019). The abundance of readily convertible nutrients and chemicals in DFW enables efficient fermentation by a range of microorganisms, especially when hydrolysis by enzymes is employed to aid the process. Regardless of its source, DFW generally contains a high amount of carbs. However, the ratio of fermentable soluble carbohydrates to complex carbohydrates that require hydrolysis might vary greatly (Di Bitonto *et al*., 2018). DFW may include substantial amounts of starch and cellulose, depending on the dietary practices of each location. Both of these components need to undergo saccharification in order to be properly fermented. Saccharification can be accomplished using chemical means (Ahmad *et al*., 2020), thermochemical techniques or enzymatic methods can be used to convert the substance by introducing amylolytic along with cellulolytic enzymes in appropriate conditions (Ben *et al*., 2019).

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 (Samuel *et al*., 2020; Ude *et al*., 2020; Marzouk *et al*., 2021; Fakhari, 2023). While RSM has been used for bioethanol production from biomass waste, 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 bioethanol production through ANN and ANFIS remains limited. Therefore, this study aims to utilize soft computing techniques to model the production of bioethanol from cassava waste slurry using the yeast *S. Cerevisiae*.

2. Materials and Methods

2.1 Bio-ethanol Production/ Process Modelling

Generally, bio-ethanol was produced in the following order: designing an experiment, collections of samples/raw material, development of inoculums, hydrolysis and fermentation, separation, and purification, as reported by Ugwuodo *et al,* 2021.This research employed the use of a PC equipped with the application MATLAB version 13 software for the design and modelling of experiments for data generation in ethanol production from waste cassava slurry. The modelling was conducted using the artificial neural network and fuzzy logic toolbox in MATLAB R2013a.

2.1.1 Physiochemical Analysis of Sample

The crude protein, ash content, total fat, moisture content, crude fibre, volatile matter, and fixed carbon of the cassava waste slurry sample was determined using methods as described by AOAC, 2008.

2.2 Soft Computing of the Bio-ethanol Production

The bioethanol production from cassava waste slurry was modelled with artificial neural network (ANN) and adaptive neuro-fuzzy inference systems (ANFIS) using a design matrix generated by Design Expert version 13. The dependent variable is ethanol yield, while the independent variables are temperature, pH, and sugar concentration, with a total of 19 experimental runs (Table 1).

2.2.1 ANN Modeling

The multi-variable-single output (MISO) neural architecture (Figure 1) was implemented to model the fermentation process. The independent variables are listed in Table 1, while the single output represents the ethanol yield. The dataset in Table 1 was triplicated, and the number of neurons was adjusted to prevent overtraining and overfitting. Consequently, fifty-seven (57) 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 39 samples, while fifteen percent was allocated for both testing and validation, with each comprising 9 samples. The model's performances were assessed with mean square errors (MSE) and the coefficients of determination.

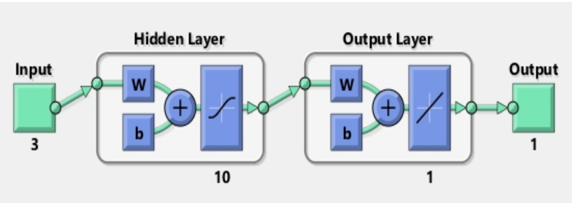

Figure 1: MISO neural architecture

2.2.2 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 bioethanol 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 modelling was conducted using the fuzzy logic toolbox in MATLAB R2013a.

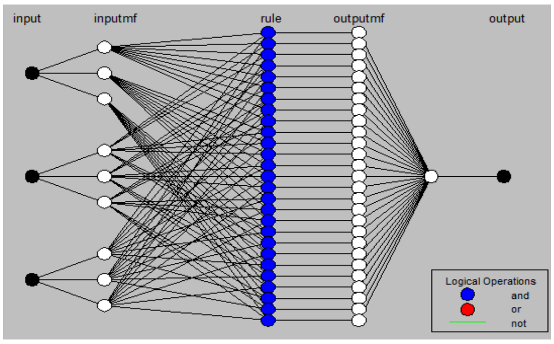

Figure 2: ANFIS architecture for bioethanol production

2.2.3 Statistical Evaluation of the models

The performance of the each model was validated by assessing statistical metrics including mean-square error (MSE), and coefficients of determination (R^2). The statistical indicators were evaluated using Equations 1-2, as outlined by Ude *et al.* (2022).

$$\text{MSE} = \left(\sum_{i=1}^{n} \frac{\text{Predicated value - Experimental value}}{n}\right) \quad (1)$$

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

2.4 Fourier transform infra-red (FTIR) spectroscopy

FTIR analysis of the distilled bio-ethanol was done to determine if peaks representing ethanol bonding were present or not and to check all the functional groups in the ethanol. This was done according to the method described by (Kim *et al.*, 2013).

3. Result and Discussion

3.1 Physiochemical Analysis Result (Proximate Analysis)

The results of the proximate analysis carried out on the sample of the cassava waste water is as shown in Table 2. The values of protein, ash content, total fat, moisture content, crude fibre, volatile matter and fixed carbon of sample A, were 0.69, 0.48, 0.55, 1.48, 86.68, 2.60, 9.98 and 2.86(%w/w) respectively. The proximate analysis results of the cassava waste water showed that the cassava waste water contain more moisture, volatile matter and fixed carbon. This results are consistent with findings from Okudoh *et al.* (2014), Onifade *et al.* (2015), Ugwuodo *et al.* (2021).

Table 2: Proximate Analysis of the cassava waste slurry (Ugwuodo *et al.*, 2021)

Item	% value
Crude protein	0.69
Ash content	1.04
Total fat	0.55
Moisture content	86.83
Crude fibre	2.90
Volatile matter	9.98
Fixed carbon	6.82

3.2 ANN Modelling of Bioethanol Production

The artificial neural network (ANN) was utilized to forecast the ethanol fermentation parameters, employing a supervised learning approach. Figure 3 illustrates the network's training performance, revealing a mean square error of 0.013488 for the prediction of bioethanol yield at a maximum epoch of 7, indicating commendable performance with minimal errors. Additionally, Figure 4 presents the model's plot for bioethanol 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 bioethanol yield. This is in line with the work of Samuel *et al.* (2020).

Table 1: Response of Experimental Design Matrix

Run	Factor 1 A:Temperature (ºC)	Factor 2 B:Sugar Conc. (mol/dm)	Factor 3 C:pH	Response 1 Experimental Yield (%)	ANN Predicted Yield (%)	ANFIS Predicted Yield (%)
1	32.5	0.2375	5.25	30	30.00	30.00
2	32.5	0.4267	5.25	46	45.99	46.00
3	40	0.35	6.5	50	49.99	49.99
4	32.5	0.2375	5.25	30	30.00	30.00
5	32.5	0.0482	5.25	34.8	34.80	34.80
6	19.89	0.2375	5.25	52	51.99	52.00
7	32.5	0.2375	3.14	38	38.00	37.99
8	32.5	0.2375	5.25	30	30.00	30.00
9	25	0.35	6.5	48	47.99	47.99
10	40	0.125	4	47	47.00	46.99
11	32.5	0.2375	7.35	34	35.92	34.00
12	32.5	0.2375	5.25	30	30.00	30.00
13	32.5	0.2375	5.25	30	30.00	30.00
14	45.11	0.2375	5.25	57	57.00	56.99
15	25	0.125	6.5	42	41.99	42.00
16	40	0.125	6.5	35	34.99	35.00
17	40	0.35	4	59	58.99	58.99
18	25	0.125	4	35	35.00	34.99
19	25	0.35	4	42	42.00	42.00

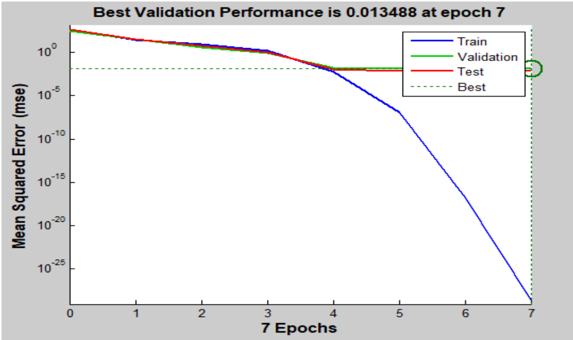

Figure 3: MISO Performance Error for Predicting of bioethanol Yield

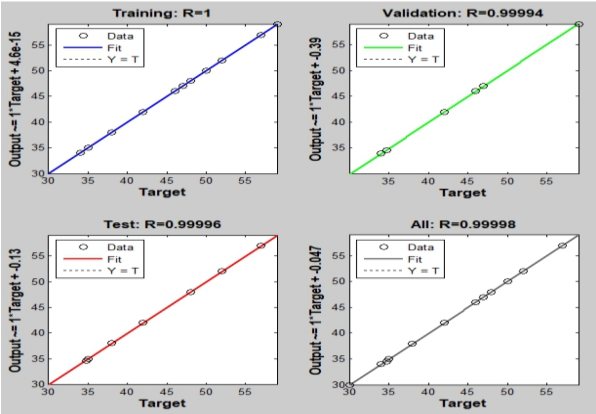

Figure 4: MISO Regression Analysis for Bioethanol Yield Prediction

3.3 ANFIS Modelling

The responses from the experimental design matrix for the production of bioethanol from cassava waste slurry were modelled using the ANFIS approach, as shown in Table 1. Figure 5 illustrates the correlation between the actual and generated yields for the ANFIS bioethanol production model. The model achieved a R^2 of 0.9999, with an error of 0.0000013607, 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 99.99% of the variability observed.

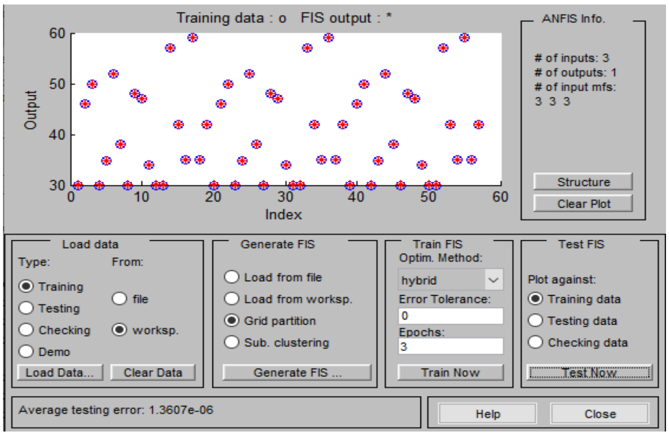

Figure 5: Experimental and predicted bioethanol yield

Additionally, surface plots were created to assess the impact of various combinations of production factors on bioethanol yield, and these are presented in Figure 6 (a-c). Specifically, Figure 6a illustrates the interactive influence of the temperature and sugar concentration on the yield of bioethanol produced from cassava waste slurry. It is evident that an increase in the reaction temperature results in an increase in the yield of the ethanol produced. Similarly, an increase in the sugar concentration also increases the yield of ethanol. This may be due to the fact that more sugars are transformed by the action of the enzymes as the temperature increases. This compared well with the report of Ugwuodo *et al*. (2021).

Figure 6b illustrates the effect of temperature and pH on the yield of ethanol. The figure revealed that an increase in the reaction temperature results in a steady and significant increase in the yield of the ethanol produced. Similarly, an increase in the pH led to a slight increase in the yield of ethanol until it reached a pH of 6.5, after which a further increase in the pH led to a corresponding decrease in the yield. This may be due to the inability to produce enough fermentation sugars. The remaining sugars are the non-fermentation fraction of the total sugars. This result is similar to that of Dadhania *et al*. (2021).

In Figure 6c, the combination of pH and sugar concentrations on bioethanol yield is depicted. It is evident from the plot that ethanol yield rises significantly with rising sugar concentration, and an increase in pH resulted in an insignificant increase in the yield of ethanol. This may be attributed to the availability of sufficient sugars to be converted. A similar trend was reported by Lucas *et al*. (2016).

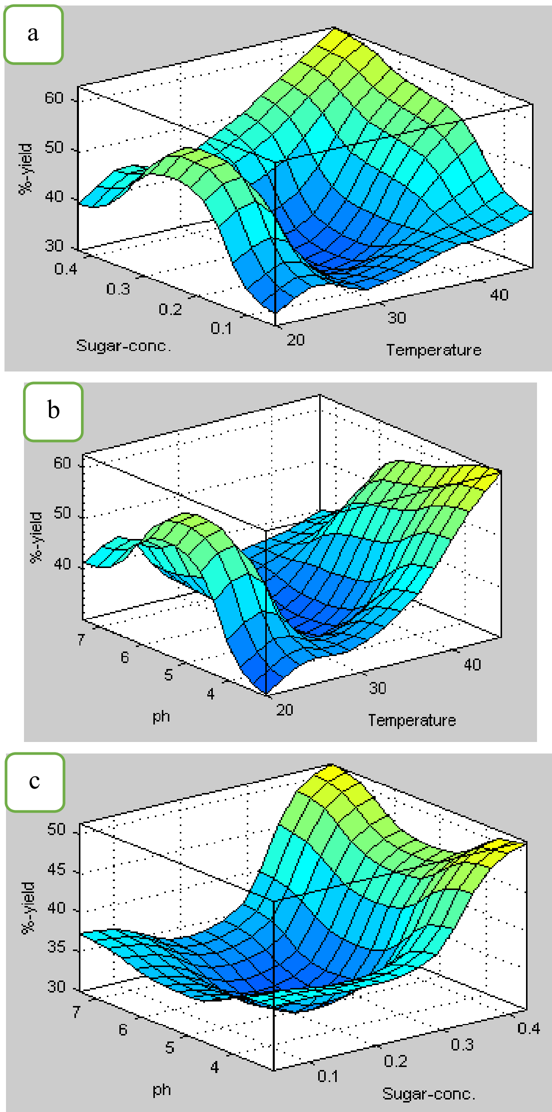

Figure 6: Surface plots of the ANFIS model for the interaction effect of (a) temperature/sugar concentration, (b) temperature/pH, and (c) sugar concentration/pH.

The optimization of bioethanol yield from cassava waste slurry was conducted through ANFIS rules, focusing on the temperature, sugar concentration, and pH. The findings indicated that a bioethanol yield of 30% from cassava waste slurry was achieved when these parameters were set to 32.5 ^oC, 0.238 mole/dm^3, and 5.25, respectively. Furthermore, the validation of the optimal yield 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.

3.4 Performance evaluation of the developed models

Statistical metrics were employed to assess the performance of the ANN and ANFIS models developed for predicting ethanol yield, with the results presented in Table 3. The R^2 values for the ANN model were almost the same as those of the ANFIS model. Moreover, the ANFIS exhibited lower error rates compared to the ANN model, and both models displayed low calculated mean squared errors (MSEs). This suggests that while the ANFIS is more effective in predicting bioethanol yield from cassava waste slurry through fermentation, with ANFIS predicting the yield of bioethanol at 99.99% and the ANN model at 99.998%, both models are viable options for estimating bioethanol yield.

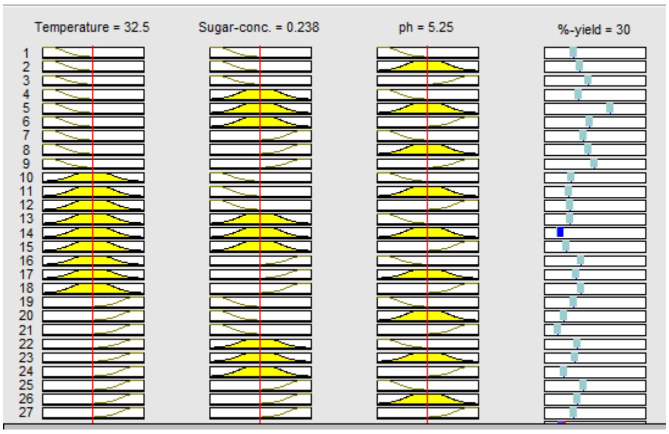

Figure 7: ANFIS rule viewer for bioethanol yield from cassava waste slurry

Table 3: Statistical Indices of the Model

Index	ANN	ANFIS
R^2	0.99998	0.9999
MSE	0.013488	0.0000013607

3.4 FTIR Analysis Result

From the Figure 8, it can be observed that the peaks became sharper and clear which is an indication of pretreatment with acid at higher concentration of H_2SO_4 which indicates that the substrate became more pure after treatment. The FTIR band at 1640.0 cm^{-1} and 1453.7 cm^{-1} signifies the presence of aromatic ring vibrations, indicating the structural characteristics of lignin to which these bands are attributed. These peaks also suggest weaker hydrogen bonding interactions commonly associated with lignin structures (Pandey and Pitman, 2003). The broad absorption peak observed at 3287.5 cm^{-1} corresponds to O–H stretching vibrations, indicating the presence of hydroxyl groups and suggesting the degradation of cellulose during the process (Sun *et al*., 2004). The peak at 2981.9 cm^{-1} is attributed to C–H stretching vibrations, which are typically associated with aliphatic chains and the disruption of ester bonds (Colom and Carrillo, 2005). The reduction of these specific chemical bonds facilitates the exposure of cellulose and hemicellulose chains, thereby enhancing enzyme accessibility and promoting higher ethanol yields during fermentation. This results agrees with the results of Mustafa, *et al*. (2019), who performed similar work using cassava waste peels.

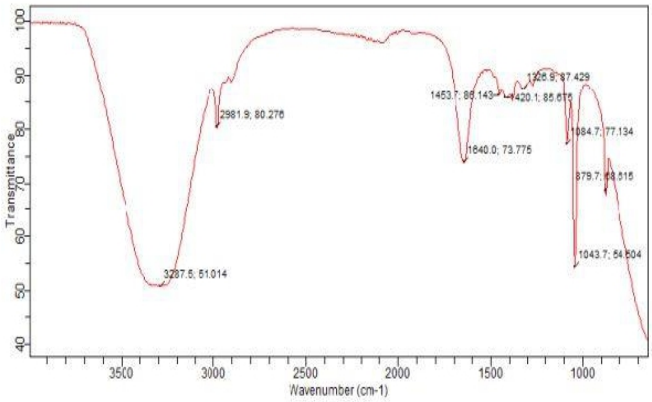

Figure 8: FTIR analysis for the distilled bio-ethanol

4. Conclusion

This study demonstrated the feasibility and effectiveness of producing bioethanol from cassava waste slurry using *Saccharomyces cerevisiae* under optimized conditions. The integration of soft computing techniques—Artificial Neural Networks (ANN) and Adaptive Neuro-Fuzzy Inference Systems (ANFIS)—enabled precise modeling and prediction of fermentation outcomes based on key process parameters: temperature, pH, and sugar concentration. Among the two models, ANFIS exhibited superior performance, achieving a coefficient of determination (R^2) of 0.9999 and minimal mean square error, highlighting its robustness and predictive accuracy. Optimal fermentation conditions (32.5 °C, 0.238 mol/dm^3 sugar concentration, and pH 5.25) yielded 30% ethanol. Additionally, FTIR analysis confirmed the structural signatures of ethanol, validating the biochemical conversion process. These findings highlight the potential of cassava waste as a low-cost, sustainable feedstock for bioethanol production and reinforce the application of AI-driven models in optimizing bioconversion processes for scalable, eco-friendly biofuel technologies.

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