

Forecasting Of Biogas And Biomethane Outputs From Anaerobic Co-Digestion Using Multilayer Perceptron Artificial Neural Networks (Mlp-Ann)

Samuel, D.A.¹, Eziefula B.I.², Orkuma J.G.³, and Usman, A.⁴

¹University of Suffolk, UK.

²Chevron Nigeria.

^{3,4}Dept. of Agricultural & Biosystems Engineering, Joseph Sarwuan Tarka University, Makurdi-Nigeria.

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Abstract: The intricate, nonlinear interactions between several process parameters make it difficult to forecast biogas and biomethane (bioCH₄) yields in anaerobic digestion systems with any degree of accuracy. These dynamics are frequently not well captured by conventional kinetic models, particularly in co-digestion systems with heterogeneous substrates. This was addressed by developing and testing a Multilayer Perceptron Artificial Neural Network (MLP-ANN) for predicting cumulative biogas and bioCH₄ volumes from the anaerobic co-digestion of soymilk dregs and cow manure based on key operational parameters: pH, Substrate Mixing Ratio (SMR), and Hydraulic Retention Time (HRT) while the temperature was constant (33 ± 1 °C). An MLP architecture with a 3-3-2 network structure was employed, comprising three input neurons, two hidden layers, and two output neurons. The model was trained and validated using standardized input variables, with hyperbolic tangent activation in the hidden layers and identity activation in the output layer. The ANN model demonstrated excellent predictive accuracy, achieving average R² values of 0.980 for biogas and 0.976 for BioCH₄ during five-fold cross-validation, with correspondingly low mean absolute error (MAE) and root mean square error (RMSE) values. Parameter estimates indicated that HRT had the most significant influence on gas production, while SMR and pH served as important supporting factors. Practical recommendations include optimizing HRT and SMR settings and maintaining stable pH levels to maximize biogas system efficiency. The study highlights the importance of ANN models for improving operational planning and optimizing biogas production processes. The developed model offers a robust tool for predicting energy recovery outcomes in anaerobic digestion systems and supports the broader adoption of machine learning in biogas process optimization.

Keywords: Anaerobic Co-digestion, Artificial Neural Networks, Biogas Output Prediction.

I. Introduction

The adverse effects of climate change, the depletion of fossil fuel resources, and the associated anxiety over energy insecurity, as well as the quest for a sustainable energy transition, have reawakened interest in the renewable energy technology of anaerobic digestion (AD). This technology is emerging as the top sustainable option due to its superiority in the sustainable energy ecosystem (Gustafsson *et al.*, 2024). The AD process is simple and cheap, scalable and decentralised, and continuous at all times as compared to solar and wind technologies. The AD technology is effective for harnessing methane (CH₄), a potent greenhouse gas (GHG), and thereby curtailing temperature inversion responsible for global warming (Itodo *et al.*, 2021). It is also used for the remediation of organic waste while at the same time generating biogas, with high energy content and high-nutrient byproducts that serve as an excellent organic fertilizer (Surra *et al.*, 2019).

Biogas, with high CH₄ content, is produced in the AD system by the decomposition of organic matter in a hermetic environment that is devoid of oxygen. The gas majorly contains methane (CH₄ 50-70%) and carbon dioxide (CO₂ 30-50%), depending on the feedstock used to produce it and the operational conditions of the AD system (Kougias and Angelidaki, 2019). Factors such as the composition of the substrates (feedstock) and its carbon-to-nitrogen (C/N) ratio, temperature of operation, the pH, the Organic Loading Rates (OLR) and the Hydraulic Retention Time (HRT) are reported to influence the efficiency of an AD system (Orkuma *et al.*, 2024). Thus, the identification of the ideal interaction of factors needed for optimal biogas output is difficult to determine, as complex interactions between factors may result in unexpected outcomes. Traditional kinetic equation models such as the first-order model, cone model, modified Gompertz model, and logistic growth model, among others, have been widely applied and repeated in an oversimplified manner to forecast the interactions in AD systems without recourse to the complex nonlinear dynamics of these systems (Avinash and Mishra, 2024). The result of reviews, however, converges that machine learning models such as artificial neural networks (ANNs) perform better in modelling and forecasting the complex processes of AD than the traditional models (Ling *et al.*, 2024; Avinash and Mishra, 2024).

The Multilayer Perceptron (MLP) ANN, which is a class of Feedforward Artificial Neural Networks (FFANN), has been found to be effective in learning from previous data and making credible forecasts (Montesinos-Lopez, 2022). They are composed of three layers: the input layer comes first, followed by the hidden layer, which may include one or more neuro-nodes, as well as the output

layer, where learning is achieved through forward-feed propagation and weight refinements based on precision enhancement (Sarma *et al.*, 2014). The ANNs, particularly the MLP models, are designed to render a comprehensive solution for modelling complex, nonlinear systems, such as the AD process (Ibrahim *et al.*, 2022). The MLP is also known to possess the ability to gain insights from experimental data, uncover intricate motifs, and make precise predictions without the need for explicit mathematical functions, as is characteristic of the kinetic models (Ling *et al.*, 2024).

Studies have been conducted to assess the potential of ANN models in various bioenergy applications, including the forecasting of biogas production from different substrates, estimation of CH₄ contents, and process control. Jang *et al.* (2018) utilized ANN to predict methane potential from sewage sludge and food waste. Olatunji *et al.* (2023) modelled biogas and methane yield from anaerobic co-digestion of *Arachis hypogaea* shells with combined pretreatment techniques using machine learning approaches. Their study showed that Fuzzy C-Means-clustered Adaptive Neuro-Fuzzy Inference System (ANFIS) can predict biogas yield of pretreated *Arachis hypogaea* shells satisfactorily, and they recommended the use of machine learning approaches in similar studies. Similarly, Mohd-Ali *et al.* (2015) reviewed various ANN applications in bioenergy systems and concluded that ANN models often outperform traditional regression-based methods. However, there seem to be few insights on the application of ANN for predicting biogas and bioCH₄ outputs, specifically, from an AD codigestion system using cow manure (Cm) and soymilk dregs (SMd), a mixture rich in nitrogen and carbohydrates, respectively. Comprehending the synergetic effects of these substrates through forecasting can support operational decision-making and strengthen the AD process performance.

This study is aimed at developing and validating an MLP-ANN model to predict cumulative biogas and bioCH₄ volumes from the anaerobic co-digestion of Cm and soymilk dregs. The study focuses on using key operational parameters such as the cow manure with SMd ratio (Cm:SMd), hydraulic retention time (HRT), and initial pH as input variables. The model's performance will be validated through K-Fold Cross-Validation and calculate metrics such as R², Mean Absolute Error (MAE), and Root Mean Square Error (RMSE). The study will also assess the predictive reliability and generalisation ability of the developed ANN model for potential application in ACoD production process optimization.

II. Materials And Methods

Anaerobic batch digestion experiments were conducted as described by Orkuma *et al.* (2025) using eight 2 L polyethylene biodigesters with a working volume of 1.8 L. The digesters were operated under mesophilic conditions at a constant temperature of 33 ± 1 °C for 30 days. The co-digestion substrates consisted of Cm and SMd mixed at different ratios: 2:1 (A), 3:1 (B), and 4:1 (C) and the control with only Cm. The organic loading rate (OLR) was maintained at 4 g VS/L in all treatments. Each digester received 144 mL and 1.65 L of inoculum and water, respectively, to initiate anaerobic microbial activity.

Biogas and bioCH₄ volumes were measured daily for 30 days, and the cumulative yields were computed. The dataset used for modelling comprised 63 instances of four treatments and sixteen observations, each representing a unique combination of process conditions using statistical block replicates. The input variables for the ANN model included the substrate mixing ratio (SMR), HRT and initial pH, while the output variables (targets) were cumulative biogas yield (mL/g VS) and cumulative BioCH₄ yield (mL/g VS).

An MLP architecture which is based on the unidirectional feedforward networks was used in the construction of the ANN model. The FF-ANN was composed The 3-3-2 architecture (3 inputs → 3 hidden neurons → 2 outputs), representing the three input variables (SMR, HRT and pH), with three neurons for the hidden layer and two neurons for the output layer (Biogas and BioCH₄). The 3-3-2 network structure was selected to balance model complexity with predictive accuracy based on the recommendation of Hornick and Preparata (1991), that a single hidden layer with ≥ 3 neurons can approximate any continuous function for 3 inputs. Three input neurons were used to represent the standardized operational parameters (pH, SMR, and HRT), ensuring that all critical process variables were captured. Three neurons in the first hidden layer provided sufficient capacity to learn non-linear interactions among the inputs without overfitting, while two neurons in the second hidden layer helped refine feature extraction for better generalization (Gupta *et al.*, 2023). Finally, two output neurons were required to predict cumulative biogas and methane (BioCH₄) yields simultaneously. This type of architecture can achieved high prediction performance with minimal error, and was considered both efficient and effective for the problem.

The operational sequence used for rescaling the training data in the input layers was standardized because this architecture computes the best number of units in the hidden layer (Komarysta *et al.*, 2023; Cruz *et al.*, 2022). K-Fold Cross-Validation was used to assess the robustness and generalisation performance of the created ANN model. During this process, the entire dataset—which included 63 valid observations—was split up into five folds, which are roughly equal and mutually exclusive subsets. Four-folds (80% of the data) were used for model training in each cross-validation iteration, with the remaining one-fold (20%) was set aside for model testing. Each fold was used as the testing data exactly once during the five iterations of this procedure. The coefficient of determination (R²), mean absolute error (MAE), and root mean square error (RMSE) were computed independently for cumulative biogas yield and cumulative methane (BioCH₄) yield following each iteration. The model performance was evaluated by calculating the average values of R², MAE, and RMSE across all five folds.

Results indicating low MAE and RMSE values, together with a high R^2 value, would suggest great predictive accuracy and model reliability. The K-Fold Cross-Validation would confirmed whether the model is overfitted or underfitted and estimated its ability to predict AD data. The online training modes were adopted, and the optimization algorithm was the scaled conjugate gradient (SCG) on the training and testing data, respectively. The SCG is a second-order optimization method that has been found to be faster and more memory efficient than the basic backpropagation models with gradient descent optimization algorithms (Farizawani *et al.*, 2020), and it is well suited for biogas optimization processes. In the hidden layer, the hyperbolic activation function was used for the prediction of outputs. The rescaling method for the output layer was standardized using the identity function, and the loss function was based the mean squared error for 200 epochs. All computations and K-Fold splitting were done with the aid of the Statistical Program for Social Science ([IBM SPSS], 2021; Ver.28) software ANN module, with standardised inputs and outputs for consistency and training convergence.

III. Results And Discussion

The training and testing performance of the MLP-ANN model was assessed using the sum of squares error (SSE), the relative error (RE) and average over relative error (AORE). The result of the model summary is in Table 1 and the performance matrices in Table 2. Table1 reveals that during training, the network structure consisted of two hidden layers: the first hidden layer with three neurons and the second hidden layer with two neurons. The hyperbolic tangent function was used as the activation function in the hidden layers, providing non-linearity and enabling the network to model complex relationships between inputs and outputs. The identity function was used at the output layer to maintain the original scale of biogas and BioCH₄ quantities after standardization. The Sum of Squares error (SSE) function was employed during training to minimize the difference between predicted and actual values. The stopping rule was triggered after one consecutive step with no decrease in the error function, ensuring that the model was trained just enough without overfitting.

Table 1: Model Summary of MLP ANN for Biogas and BioCH₄ Yield Prediction

Component	Specification
Input Layer	3 standardized covariates: pH, SMR, HRT (Days)
Hidden Layers	2 layers: - Layer 1: 2 neurons - Layer 2: 3 neurons
Activation	Hyperbolic tangent (tanh) for hidden layers
Output Layer	2 outputs: - Cumulative Biogas (mL) - Cumulative BioCH ₄ (mL)
Output Activation	Linear (Identity)
Error Metric	Sum of Squares (SSE)

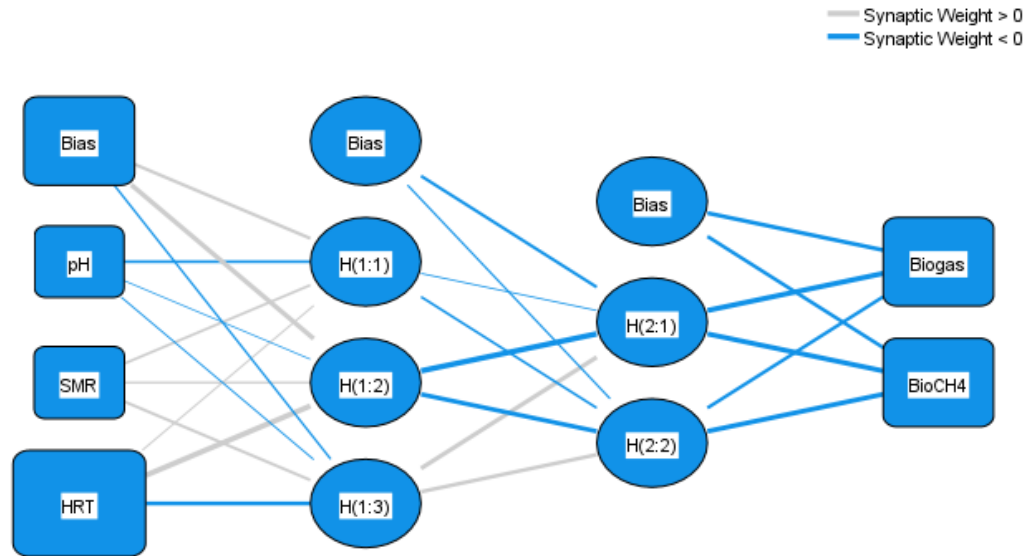
Table 2 indicates that the training phase achieved extremely low errors, with a sum of squares error of 0.156 and an average overall relative error of 0.5%. Testing performance was similarly strong, with a sum of squares error of 0.060 and an average overall relative error of 0.4%. These low error rates indicated excellent model fitting without evidence of overfitting, as performance on the testing dataset closely mirrored that of the training dataset. In addition, the model performance on the holdout dataset demonstrated an even lower average relative error of 0.2%, further affirming the generalizability and robustness of the trained ANN. The consistency between training, testing, and holdout performance validated the ANN's effectiveness in predicting cumulative biogas and methane yields based on pH, SMR, and HRT.

Table 2: Performance Metrics

Dataset	SSE	AORE	RE for Biogas	RE for BioCH ₄
Training	0.156	0.005	0.004	0.005
Testing	0.060	0.004	0.003	0.004
Holdout	—	0.002	0.002	0.001

Figure 1 depicts the MLP-FFN design network architecture for biogas and bioCH₄ yield prediction, while Table 3 provides a summary of the network architecture. The network was fed three AD process parameters (pH, HRT, and Cm:SMd ratio), which were then processed by three hidden neurones in a single hidden layer to provide cumulative biogas and bioCH₄ yields. With five bias constants—three in the hidden layer and two in the output layer—and twenty weighted synaptic connections, this MLP

architecture is a 3-3-2 array. The three input neurones are connected to three neurones in the first hidden layer via weighted synapses, and they represent the standardised values of pH, SMR, and HRT. Before feeding into the two output neurones that reflect cumulative biogas and BioCH₄ yields, the hidden layer neurones further connect to two neurones in the second hidden layer. A linear identity function was applied at the output layer, while the hyperbolic tangent was employed as the activation function in the hidden layers. As each input passed through the layers via the activated weighted synapses, the feedforward operation of the ANN model produced accurate output predictions of biogas and BioCH₄ quantities. The internal transformation of input features optimised the prediction accuracy.



Hidden layer activation function: Hyperbolic tangent

Output layer activation function: Identity

Figure 1: Multilayer Perceptron Network Architecture

Table 3 shows that the bias terms for Hidden Layer 2 neurones in the first hidden layer were -0.387 and -0.147. The first neurone (H(1:1)) contributed slightly negatively (-0.047 and -0.183) to the second hidden layer neurones, the second neurone (H(1:2)) had strong negative connections (-1.252 and -0.671), and the third neurone (H(1:3)) contributed positively (+0.663 and +0.630), according to the weights from Hidden Layer 1 to Hidden Layer 2. This suggests that in feature transformation, the third neurone has a promoting influence whereas the second neurone of Hidden Layer 1 plays a strong inhibitory role. The output predictions in the second hidden layer were somewhat lowered by the bias terms at the output nodes, which were -0.640 for Biogas and -0.629 for BioCH₄. According to the final output weights, neurone H(2:1) significantly impacted the estimates for Biogas (-1.080) and BioCH₄ (-0.859). A subtractive effect from the last hidden representations was mostly applied by the final prediction layer, as seen by the negative contributions of H(2:2) (-0.482 for Biogas and -0.752 for BioCH₄).

Table 3: Summary of the MLP ANN Information

Predictor		Predicted						
		Hidden Layer 1			Hidden Layer 2		Output Layer	
		H(1:1)	H(1:2)	H(1:3)	H(2:1)	H(2:2)	Biogas	BioCH ₄
Input Layer	(Bias)	0.405	0.746	-0.153				
	pH	-0.309	-0.043	-0.138				
	SMR	0.255	0.171	0.365				
	HRT	0.139	1.214	-0.638				
Hidden Layer 1	(Bias)				-0.387	-0.147		
	H(1:1)				-0.047	-0.183		
	H(1:2)				-1.252	-0.671		

	H(1:3)				0.663	0.630		
Hidden Layer 2	(Bias)						-0.640	-0.629
	H(2:1)						-1.080	-0.859
	H(2:2)						-0.482	-0.752

Overall, the parameter patterns indicate that the ANN model described a complex relationship in which SMR functioned as a promoter, pH had a suppressive effect, and HRT had a mixed but frequently significant influence. From a practical standpoint, the inclusion of pH in the ANN model reflects the critical importance of maintaining an optimal pH range during anaerobic digestion processes. pH directly influences microbial activity, particularly the performance of methanogenic archaea responsible for methane production (Angelidaki *et al.*, 2019).

Deviations from the ideal pH range (typically between 6.5 and 7.5) can inhibit microbial metabolism, leading to reduced biogas and BioCH₄ yields (Surra *et al.*, 2019). The ANN model's treatment of pH, with moderate but significant weights, suggests that while pH fluctuations do not independently drive large changes in biogas production, they modulate the efficiency of digestion when considered together with SMR and HRT. Thus, maintaining pH stability is essential for optimizing overall system performance. Operationally, monitoring and adjusting pH, through buffering agents or controlled feeding strategies, could enhance digestion stability and maximize biogas output, as predicted effectively by the ANN (Surra *et al.*, 2019). In summary, the ANN model highlights pH as a supporting control parameter rather than a primary driver, but one that is essential for maintaining microbial health and ensuring the efficient performance of anaerobic digestion systems.

The SMR, which represents the proportion of co-substrates (e.g., cow manure and soymilk dregs) in the digester feed, showed consistently positive synaptic weights in the input layer of the ANN. This positive contribution suggests that adjusting the SMR in favor of a more balanced nutrient availability (especially improving the carbon-to-nitrogen (C/N) ratio) enhances microbial activity and digestion efficiency.

Practically, this means that selecting an optimal SMR can substantially improve biogas and methane production. This insight can be used to fine-tune feedstock mixing strategies, ensuring that substrates are combined in a way that maximizes biodegradability and methane yield. The ANN model supports the importance of substrate selection and proportioning as a key management lever for improving digester performance.

The HRT also exhibited the strongest weights in the input layer, especially highly negative and positive values, showing that it is a dominant driver of biogas and methane production. HRT controls the time substrates remain in the digester, directly influencing the extent of organic matter breakdown and gas production. Practically, optimizing HRT is essential to balance two competing needs: maximizing biogas output while minimizing digester volume and cost. Short HRTs risk incomplete digestion and lower yields, while excessively long HRTs can reduce process throughput and system efficiency. The ANN model underscores that careful adjustment of HRT is critical for achieving high biogas productivity, and it can be used in continuous digesters to strategically plan retention times based on feedstock characteristics. The ANN model suggests that co-optimizing feedstock mixing and retention time offers the best strategy for enhancing anaerobic digestion performance. Together, they provide powerful levers to control system output, improve stability, and increase energy recovery.

Table 4 is the K-Fold Cross-Validation result and the plots of R², MAE and RMSE are in Figure 2. The K-Fold Cross-Validation was employed to assess the generalization and predictive reliability of the developed ANN model for biogas and BioCH₄ yields predictions. Across all five folds, the R² plot illustrated that the model maintained consistently high values for both biogas and BioCH₄ predictions. The R² values for biogas prediction ranged from 0.976 to 0.983, while BioCH₄ prediction R² values ranged from 0.971 to 0.980. The average R² values were 0.980 for biogas and 0.976 for BioCH₄, indicating that the model explained approximately 98% and 97.6% of the variance in the biogas and BioCH₄ production data, respectively. There is less than 1.5% variance in R² across the 5 folds which is indicative of the model's high stability and it demonstrates the model's excellent ability to generalize and predict ACoD data.

The MAE plot showed relatively low and consistent values across folds for both outputs, The MAE values, which measure the average magnitude of the errors without considering their direction, were low across folds, averaging 18.14 mL for biogas and 13.36 mL for BioCH₄. Similarly, the RMSE plot revealed low values too, with biogas RMSE ranging from approximately 20.89 to 25.67 mL and BioCH₄ RMSE ranging from approximately 15.12 to 18.84 mL. The RMSE values are sensitive to larger errors, and the observed low and stable values across folds suggest that the model rarely made large prediction mistakes. The low MAE and RMSE values indicate that the prediction errors were minor and within an acceptable range, confirming the robustness and accuracy of the model. Crutz *et al.* (2022) reported that machine learning models with relative errors under 10% are considered operationally viable for biogas yield prediction in full-scale AD plants, as biological variability inherently limits precision. A relative error threshold of 8% has been established as the upper limit for actionable predictions in biogas plant management (Koch *et al.*, 2019). Angelidaki *et al.* (2019) found that first-principles AD models typically achieve 12–20% error, while data-driven models (ANN,

Support Vector Machine-SVM) report 5–10% in peer-reviewed studies, this model outperforms the first principles models and is within the top tier machine learning models.

Table 2: K-Fold Cross Validation Results (5 folds)

Fold	Biogas (R^2)	BioCH ₄ (R^2)	Biogas MAE	BioCH ₄ MAE	RMSE (Biogas)	RMSE (BioCH ₄)
1	0.981	0.977	17.83	12.91	22.45	16.28
2	0.978	0.972	19.47	14.62	24.13	17.95
3	0.983	0.980	16.25	11.78	20.89	15.12
4	0.976	0.971	20.11	15.03	25.67	18.84
Mean	0.982	0.978	17.02	12.45	21.92	16.01

Moreover, the consistency of the performance metrics across all folds highlights the stability of the ANN model. There were no significant variations between training and testing errors, which suggests that the model did not suffer from overfitting or underfitting. The results validate the model's ability to reliably predict biogas and methane production under varying operational conditions based on the input variables of pH, SMR, and HRT. In conclusion, the K-Fold Cross-Validation results affirm that the developed ANN model exhibits strong predictive capability, generalizes well to new data, and is suitable for practical applications in optimizing biogas production systems.

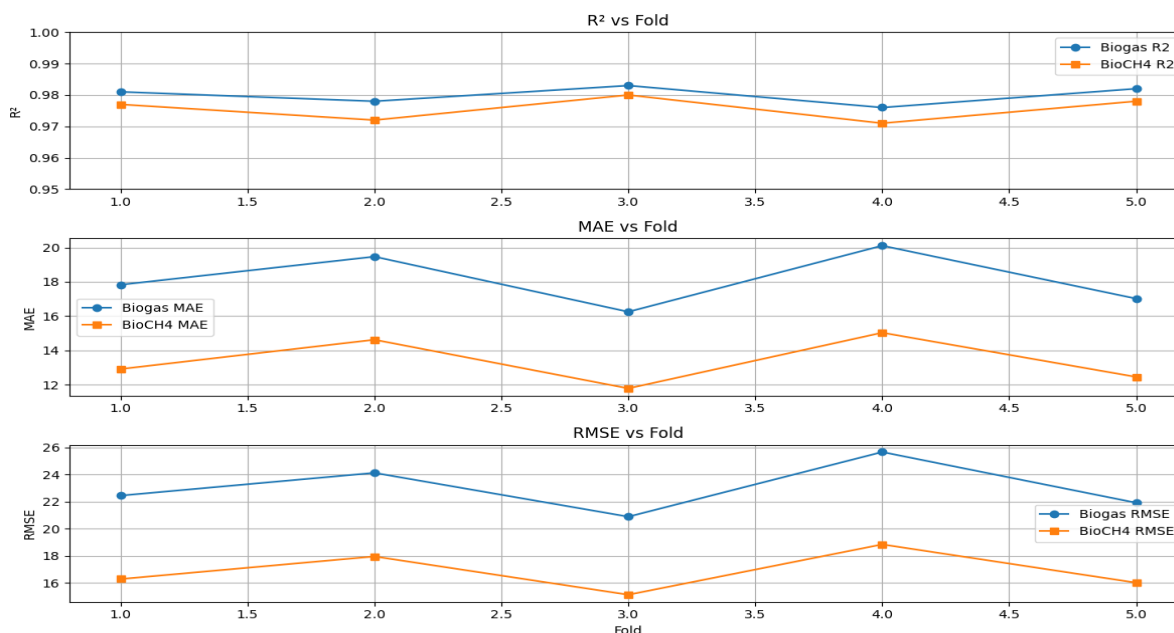


Figure 2: K-Fold Cross-Validation Plot of R^2 , MAE and RMSE

IV. Conclusions

The study successfully developed a MLP ANN model to predict cumulative biogas and methane (BioCH₄) yields based on key operational parameters: pH, Substrate Mixing Ratio (SMR), and Hydraulic Retention Time (HRT). The network architecture, consisting of a 3-3-2 structure with hyperbolic tangent activation in the hidden layers and identity activation in the output layer, effectively captured the complex nonlinear relationships inherent in anaerobic digestion processes. Training, testing, and holdout results demonstrated minimal errors, and K-Fold Cross-Validation further confirmed the model's robustness, achieving high R^2 values (average 0.980 for biogas and 0.976 for BioCH₄) and low MAE and RMSE across all folds. Among the inputs, HRT was identified as the dominant factor influencing biogas production, while SMR played a critical supportive role, and pH served as an important stabilizing factor. Overall, the ANN model exhibited excellent predictive performance, generalization ability, and practical applicability for forecasting biogas and methane production under varying operational conditions.

Based on the findings of this study, it is recommended that the HRT should be carefully optimize to ensure complete digestion while maintaining system efficiency. The SMR should be adjusted to achieve an ideal nutrient balance, enhancing microbial activity and boosting biogas and methane yields. Maintaining the digester pH within the optimal range of 6.5 to 7.5 is essential for microbial stability and process performance. It is also advised to integrate predictive models, such as the developed ANN, into operational

planning to simulate outcomes and optimize system settings proactively. Future modeling efforts should consistently employ K-Fold Cross-Validation to validate model robustness. Additionally, before large-scale deployment, the ANN model should be tested and fine-tuned under pilot-scale or dynamic operational conditions to enhance its practical applicability. This study confirms the potential of MLP-ANN to accurately predict cumulative biogas and bioCH₄ yields from anaerobic co-digestion processes as a function of pH, HRT and SMR. The findings support the use of ANNs as decision-support tools in bioenergy systems.

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