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Predicting Biogas Yield after Microwave Pretreatment Using Artificial Neural Network Models: Performance Evaluation and Method Comparison

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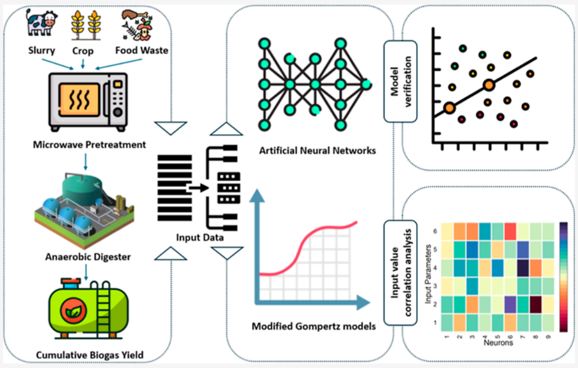

ABSTRACT: In the field of anaerobic digestion (AD) for biogas production, accurately predicting biogas yields following microwave pretreatment (MP) remains a significant challenge. Traditional kinetic models, such as the modified Gompertz (MG) model, are widely utilized but often lack the precision and adaptability needed for optimal process design and operational efficiency. This highlights a crucial gap in the development of more accurate and flexible predictive tools. To address this gap, advanced machine learning techniques, specifically, artificial neural networks (ANN), have been explored. This study developed and evaluated three ANN models: ANN, deep feed forward backpropagation (DFFBP), and deep cascade forward backpropagation network (DCFBP). The DCFBP model demonstrated superior predictive accuracy with a high coefficient of determination (R^2 = 0.9946) and a lower mean absolute error (MAE = 0.34). Key input parameters, including the ratios of volatile solids to total solids (VS/TS) and the ratio of soluble chemical oxygen demand to total chemical oxygen demand (SCOD/TCOD), were integrated to enhance the prediction precision. These findings highlight the potential of ANN models to improve biogas yield predictions, offering significant benefits for the optimization and design of AD processes.

KEYWORDS: *artificial neural networks, biomethane potential tests, kinetic model, anaerobic digestion, biogas production*

1. INTRODUCTION

In the face of rapidly depleting fossil fuel reserves and escalating greenhouse gas emissions over the past two decades, there has been a marked increase in interest toward sustainable and cost-effective renewable energy sources.[1] Biomass conversion processes have garnered significant attention in this situation, not only for their potential to replace nonrenewable energy sources but also for their ability to add value to waste and improve the economic viability of various processes.[2] Biomass, including agricultural waste, municipal solid waste, and other sources like energy crops, agricultural and forestry residues, and industrial wastes, presents an abundant feedstock to produce chemicals, fuels, and energy.[3] This diversification inspires a shift toward bioeconomy. Bioenergy, clean and renewable energy derived from biomass and waste, plays a pivotal role in this transition. It is produced through biochemical, biological, and thermochemical processes and is expected to contribute about 14%[4] to the global energy demand. Among the methods for biomass energy conversion, anaerobic digestion (AD) is emerging as one of the most efficient and promising technologies for biogas production, offering a partial but significant replacement for fossil resources in the production of chemical compounds, energy, and fuel.[5,6]

AD is a multifaceted process involving stages like hydrolysis, acidogenesis, acetogenesis, and methanogenesis, where microorganisms degrade organic substrates in an oxygen-free environment, producing biogas primarily composed of methane (50%−70%) and carbon dioxide (20%−35%).[7−9] Despite its potential for sustainable energy production and waste management, AD's efficiency is often limited by the slow breakdown of complex organic materials.[10] Microwave pretreatment (MP) addresses this issue by disrupting the cellular structure of organic materials, enhancing biogas yield, and reducing digestion time (DT).[11,12] Studies have shown a 50% increase in biogas production with MP and improved performance in the codigestion of sludge and food waste.[13,14] Additionally, the digestate from AD serves as a valuable biofertilizer, enhancing soil fertility and promoting a closed-

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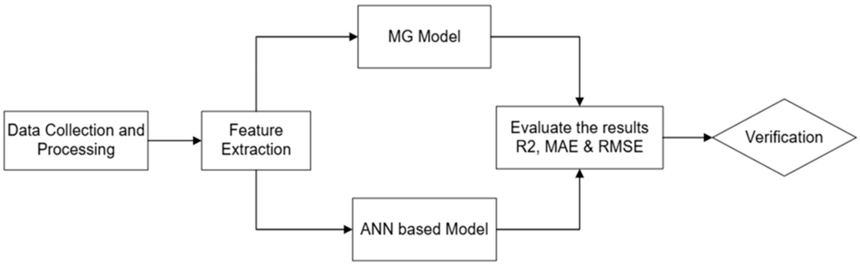

Figure 1. Methodology process: from data collection to validation.

Table 1. Comprehensive Information Regarding the Data Collection

case no.	I	II	III	IV	V	VI
sludge type	thickened waste activated sludge with fat, oil, and grease	waste activated sludge	thickened waste activated sludge	waste activated sludge and food waste	model kitchen waste	vegetable residues with mature cow dung
number of samples	9	6	12	3	3	6
experimental site	Canada	Egypt	Canada	China	Canada	Mauritius
input						
- microwave power level (W)	1250	500−1000	625−1250	600	1020−1380	87.5−350
- sample volume (ml)	200	85	350	400	75	450
- the temperature reached after microwave pretreatment (°C)	95−175	46−96	50−96	85−165	175	60−250
- VS/TS (%)	71.7−75.7	79.7−83.3	65.8−69.5	53−95	70−95	90.8−95.2
- SCOD/TCOD (%)	30.9−42.6	11.5−60.6	12−20.3	1.87−21.8	53.4−55.5	16.9−28.2
- DT (days)	38	43	35	35	21	40
output						
- CBY (mL)	925.06−1505.76	126−273	1050−2250	1760−3040	1100−1800	610−700
ref.	28	18	31	13	30	29

loop waste management system.[15] Integrating MP into AD optimizes biogas production, maximizing the potential of this renewable energy technology.[16]

Numerous mathematical models exist for predicting the outcomes of the AD process, each reflecting the intricate nature of AD. These models, ranging from the modified Gompertz (MG) equation[17] to logistic[18] and first-order equations,[19] are grounded in a combination of theoretical, analytical, and statistical methods. They serve diverse purposes, such as elucidating the AD process,[20] predicting biogas production,[16] and addressing issues like process inhibition and gas−liquid mass transfer.[21] However, a common hurdle with these traditional models is their complexity, often requiring extensive experimental data and prior knowledge for accurate predictions.[22] This complexity sets the motivation for exploring more adaptive and potentially less cumbersome alternatives like artificial neural networks (ANN), which offer a promising avenue for simplifying and improving the accuracy of AD process modeling.[23] ANN, with their ability to learn and adapt from data, could address the limitations of traditional mathematical models, paving the way for more efficient and user-friendly predictive tools in AD technology.

ANN technology has been effectively utilized as a control, estimation, and forecasting tool for AD systems and biogas production. For example, Haffiez et al.[24] developed an ANN model to predict biogas yield from an anaerobic hybrid reactor, incorporating parameters such as pH, alkalinity, organic loading rate, and chemical oxygen demand. Similarly, Yetilmezsoy et al.[25] advanced this approach by creating a three-layer ANN model, specifically for predicting biogas and methane production rates in a pilot-scale, mesophilic up-flow anaerobic sludge blanket reactor processing molasses wastewater. Further contributing to the field, Oloko-Oba et al.[26] assessed the efficacy of three distinct biodigesters for biogas production, optimizing them through an ANN model that demonstrated remarkable accuracy in biogas production prediction. Additionally, Beltramo et al.[27] introduced a swift and effective method to analyze and forecast biogas production rates using ANN. This method uniquely integrates 15 process variables from a German agricultural biogas plant and employs ant colony optimization along with genetic algorithms for variable selection, achieving a prediction error of just 6.24% and a coefficient of determination (R^2) of 0.9. These diverse applications of ANN technology in biogas production underscore its versatility and precision, marking significant advancements in sustainable energy research.

This study addresses a notable gap in the existing literature on the application of ANN technologies in forecasting biogas production using MP. Despite the well-documented effectiveness of ANN in modeling various AD processes, few studies have explored the specific use of ANN techniques for predicting biogas production enhanced by MP. This research introduces three innovative ANN models: the standard ANN model, the deep feedforward backpropagation (DFFBP) model, and the deep cascade forward backpropagation network (DCFBP) model. These models are designed to precisely predict cumulative biogas yield (CBY) from the AD of diverse organic wastes treated with MP. These models are distinguished by their integration of critical input variables, including microwave power level, sample volume, post-MP temperature, ratio of volatile solids to total solids (VS/TS), ratio of soluble chemical oxygen demand to total chemical oxygen demand (SCOD/TCOD), and digestion time (DT). Furthermore, this study presents the development of kinetic models based on the MG equation to enhance the prediction accuracy of CBY. The novelty of this approach lies in the

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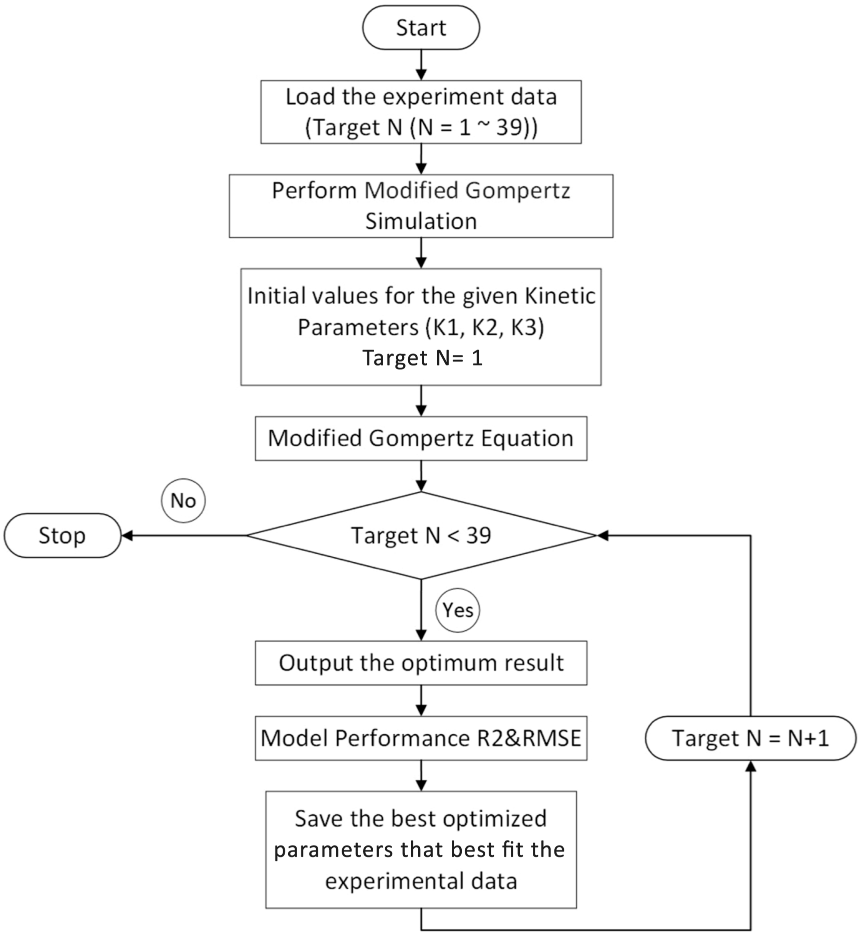

Figure 2. Flowchart of the MG model.

methodologies and their validation through key statistical performance metrics, such as R^2, mean absolute error (MAE), and root mean square error (RMSE), highlighting the potential of these innovative techniques to significantly improve predictions in AD processes.

This work builds on previous studies by integrating advanced ANN techniques with microwave pretreatment to enhance the biogas yield predictions. Unlike earlier models, which often focused on specific parameters or used conventional prediction methods, this study offers a comprehensive approach by developing and comparing multiple ANN models tailored to diverse organic wastes. By comparing the performance of ANN-based models with that of traditional kinetic models, this research highlights the advantages of ANN techniques in terms of predictive accuracy and adaptability. By addressing the limitations of existing models and demonstrating the superior predictive power of ANN techniques, this research contributes uniquely to the field of sustainable energy, offering practical implications for improving AD process efficiency and biogas yield.

2. MATERIALS AND METHODS

This section comprises three main parts: data collection and processing, model selection and development, and verification, as shown in Figure 1. It details the meticulous methods employed to gather and prepare the data, ensuring the accuracy and integrity essential for the study. The selection and construction of various predictive models are discussed, outlining the criteria and processes for developing the most suitable models to achieve the study's objectives.

2.1. Data Collection and Processing. This research paper compiles and analyzes 39 samples from various published studies[13,18,28−31] that employ microwave pretreatment to augment AD processes, as shown in Table 1. The rationale for the inclusion of these specific investigations stems from their collective emphasis on leveraging MP as a pivotal technique to enhance AD outcomes. Furthermore, these studies were chosen due to their methodological congruence, offering a coherent and comparative framework for analyzing the efficacy of MP within AD systems.

To ensure the validity and consistency of the results, we selected studies whose experiments were conducted on a laboratory scale. The change in SCOD is a significant indicator of MP's effect on organic wastes, and the TS/VS ratio[32] directly reflects the type of organic waste. Therefore, the SCOD/TCOD and VS/TS ratios are key factors in reflecting waste changes. Additionally, MP conditions can affect the CBY.[33] Consequently, the inputs for the ANN model include microwave power level and post-MP temperature to control MP conditions, SCOD/TCOD and VS/TS ratios post-MP to characterize the substrate, and sample volume and DT to assist the model in identifying different initial experimental conditions.

2.2. Model Selection and Development. In this study, two distinct methodologies were employed to develop models for predicting the CBY: the ANN-based models and those

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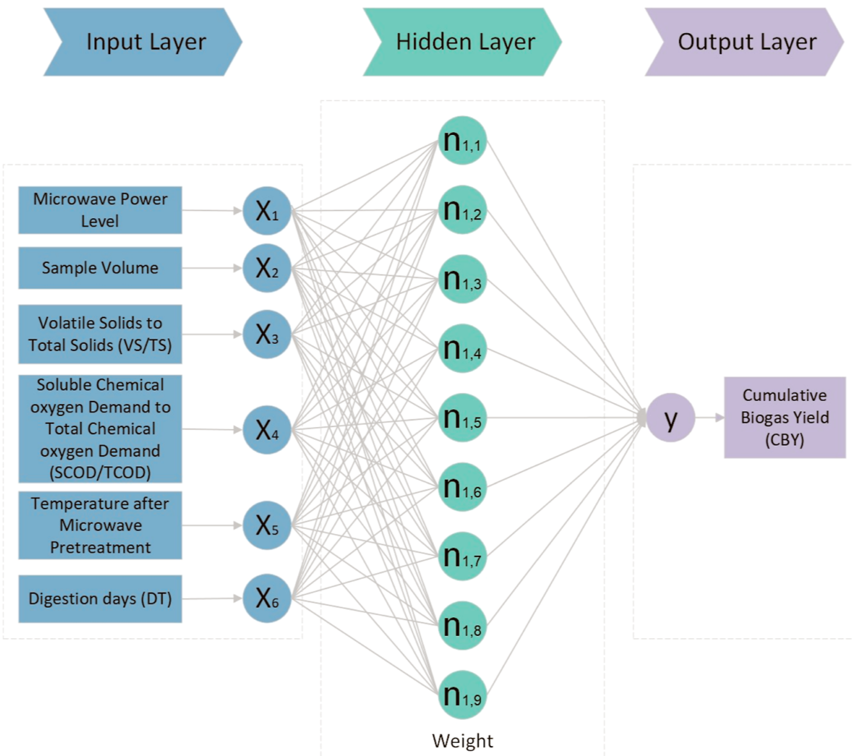

Figure 3. Architecture of the artificial neural network.

based on the modified MG equation. The latter served primarily as comparative analysis to confirm the accuracy of the ANN models. Model development began with comprehensive data preprocessing to ensure optimal quality and readiness for analysis. This initial phase was followed by the training, testing, and validation of the ANN models, which are essential for verifying their accuracy and reliability. In parallel, the kinetic parameters for the MG model were precisely determined. All processes were executed using MATLAB software.

2.2.1. MG Model. Kinetic modeling is a recognized method for describing specific system performance parameters.[34] Various kinetic models, such as the MG model,[35] the modified Logistic model[36] and the modified Richards model,[37] have been employed to simulate the AD processes and to predict the accuracy and complexity of biogas production rates. Of these, the MG model has been acknowledged as the most appropriate for representing experimental data, with an average difference between measured and predicted gas yield of only 0.76%, indicating a highly accurate model performance.[38] Membere and Sallis.[39] utilized both the Gompertz and Logistic models to investigate the effect of temperature on the kinetics of biogas production. Their results indicate that the Gompertz model not only fits the kinetics of methane production, lag time determination, and maximum methane potential but also outperforms the Logistic model with a lower RMSE of 5.45 compared to 10.23, respectively, showcasing its effectiveness. Ebrahimi-Nik et al.[40] explored the impact of drinking water treatment sludge as a mixture additive on biogas and methane production from food waste. Their findings demonstrate that the experimental biogas data fitted with the MG model, exhibiting an R^2 of 0.994, is superior to the first-order kinetic models, which displayed an R^2 of 0.949.

Consequently, this research utilizes the MG to predict CBY. eq 1 presents the modeling formulation applied for the MG equation, used for evaluating the kinetic and performance parameters of the biogas production process.

$$Y(t) = A\bullet\exp\left[-\exp\left(\frac{\mu_m \bullet e}{A}(\lambda - t) + 1\right)\right] \tag{1}$$

where $Y(t)$ is the biogas accumulation (ml/g), A is production potential (ml/g), t is the DT (day), μ_m is the maximum biogas production rate (ml/(g day)), λ is the lagging time required to produce biogas (day), and e is Euler's number (approximately 2.71828).

Figure 2 delineates the revised process for the MG model used in simulating biogas production. The procedure begins with loading the experimental data, covering a range of data sets from Target $N = 1$ to 39. A MG simulation is performed next, with initial kinetic parameters (K_1 = A (production potential), $K_2 = \lambda$ (lagging time required to produce biogas), and $K_3 = \mu_m$ (maximum biogas production rate)) set for the first data set. The simulation employs the MG Equation to process each data set. A decision point checks if all 39 data sets have been processed by evaluating if Target $N < 39$. If not, Target N increments by 1, and the model revisits the simulation step for the next data set. Once all data sets are processed, the model outputs the optimum result and assesses the model's performance using R^2 and RMSE metrics. Finally, the model saves the best optimized parameters that most accurately fit the experimental data, indicating the simulation process. This systematic approach allows for iterative analysis and optimization of each data set, ensuring precise modeling of biogas production.

2.2.2. Artificial Neural Networks Based Model. In this research, three different models for predicting CBY were developed based on the ANN model: the ANN model, the

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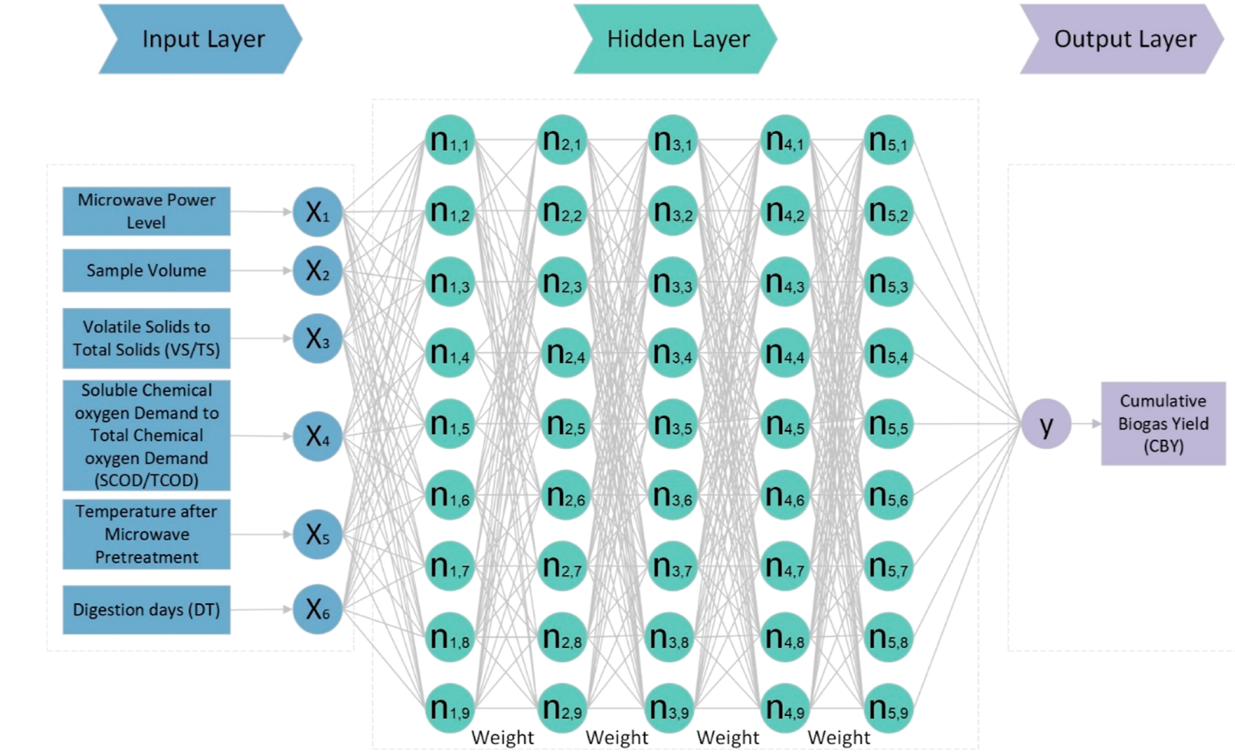

Figure 4. Architecture of deep feed forward backpropagation.

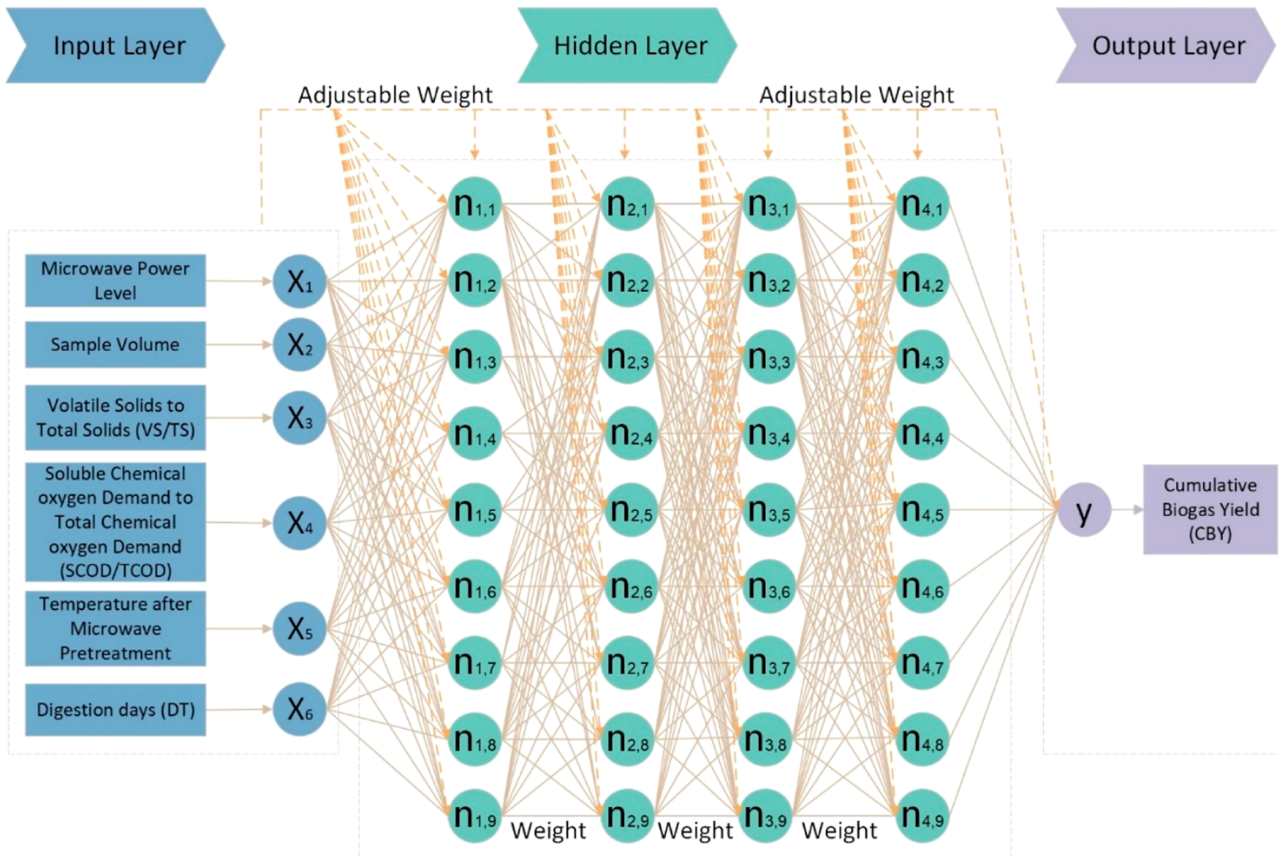

Figure 5. Architecture of deep cascade forward backpropagation.

DFFBP model, and the DCFBP model. The ANN model is a computational learning system designed to establish relationships between specific sets of input and output data.[41] This approach involves forming a mathematical model that links input and output variables without relying on pre-existing physical knowledge.[42] The structure of the ANN model is

Table 2. Optimized Parameters for the MG Model

case no.	experiment no.	K_1	R^2	K_2	K_3	maximum error (%)	no. of Iterations	MAE	RMSE
I	1	967.74	0.94	1.44	56.7	15.46	124	20.37	23.81
	2	968.48		1.8	64.51	10.06	139	22.96	24.99
	3	1057.78		0.84	61.61	5.68	123	23.48	26.31
	4	881.33		1.14	69.17	16.17	132	21.63	25.71
	5	937.73		1.88	68.2	13.13	130	20.74	26.83
	6	954.01		1.8	56.05	12.95	127	20.57	26.29
	7	1294.07		2.45	75.46	19.17	135	31.9	40.41
	8	1341.34		0.73	78.5	14.74	131	38.69	46.76
	9	1484.04		0.32	83.09	5.36	141	40.69	52.3
II	10	142.57	0.96	0.82	11.27	5.26	92	2.01	2.38
	11	159.23		1.02	12.93	0.13	92	1.81	2.11
	12	179.45		0.89	14.02	0.21	95	2.22	2.73
	13	211.82		0.86	16.91	26.05	97	2.42	3.34
	14	227.2		0.83	16.58	30.04	92	2.98	3.81
	15	276.6		0.78	19	0.49	92	2.83	3.98
III	16	2000.18	0.97	0.56	182.29	0.06	183	32.27	41.65
	17	2188.41		1.11	190.93	22.29	184	27.42	34.09
	18	2294.43		0.57	184.93	1.97	205	37.49	43.86
	19	1073.98		0.39	100.02	0.71	235	27.45	31.95
	20	1142.57		0.22	110.98	0.27	250	11.75	15.31
	21	1207.94		0.32	108.37	0.21	215	11.35	15.03
	22	2044.53		0.32	180.57	0.33	211	26.55	32.55
	23	2234.61		1.13	194.83	0.08	196	17.93	24.26
	24	2319.39		0.63	188.58	0.34	222	29.38	35.06
	25	1033.71		0.34	98.87	0.49	223	26.08	30.51
	26	1141.01		0.2	106.79	0.4	199	12.68	15.51
	27	1176.49		1.02	120.91	8.32	208	15.88	19.77
IV	28	3171.09	0.83	3.87	264.98	0.91	223	58.89	80.98
	29	3328.12		3.53	280.44	0.87	211	66.8	88.12
	30	3487.16		3.34	286.63	8.57	189	65.72	90.26
V	31	289.74	0.87	3.65	24.2	5.81	124	21.97	45.78
	32	309.7		2.96	30.74	10.67	139	24.36	51.11
	33	316.6		3.27	28.87	5.89	146	26.1	51.62
VI	34	559.46	0.97	6.34	17.56	5.13	111	8.29	10.14
	35	605.62		6.52	19.32	8.17	120	8.68	10.75
	36	622.14		6.18	20.17	26.92	148	8.38	10.17
	37	725.42		6.17	23.7	7.13	124	8.57	10.59
	38	837.24		5.93	26.84	14.18	125	11.55	13.6
	39	761.1		7.1	27.08	4.37	136	11.13	12.25

shown in Figure 3; it comprises numerous neurons distributed across the input, hidden, and output layers.[43] Each neuron in the input layer represents an independent variable and is connected to those in the hidden layers through weights (w_{ij}).[22] These weights define the strength of the input data associated with each node and are combined with a bias (b_j) to regulate the input data's magnitude (as shown in eq 2).

$$y = f\left(\sum_j w_{ij}x_{ij} + b_j\right) \quad (2)$$

Calculated values are compared with experimental values to determine the error, which is then relayed back to the input layer. To reduce this error, the weights and biases of each neuron are continuous updated throughout the training phase. These adjustments are made using a training algorithm, persisting until the discrepancy between the calculated and experimental values is reduced to the lowest feasible level. Upon the successful completion of the training, the ANN model undergoes testing with an unseen data set (test data), serving to verify the model's ability to predict accurately.

The DFFBP model extends the basic structure of the ANN by incorporating multiple hidden layers, which enhance its ability to capture complex patterns in the data.[44] Figure 4 illustrates the internal architecture of the DFFBP model. Each layer in the model processes outputs from the previous layer, applying a nonlinear activation function to learn hierarchical representations of the data. This model is particularly effective for problems where the relationships between input and output are intricate, requiring deeper computational layers for accurate predictions.

In contrast, the DCFBP model introduces additional connectivity compared to traditional feedforward architectures. Figure 5 shows the internal architecture of the DCFBP. In this model, each neuron receives inputs from not only the previous layer but also all preceding neurons in the network. This architecture allows for more complex patterns to be learned more effectively because it can capture both deep and broad data dependencies.[45] The cascade structure enhances the network's ability to adapt and learn from large data sets,

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making it highly suitable for dynamic environments where relationships between variables may change over time.

Future sections of this paper will explore the comparative performance of the models on a comprehensive data set derived from 39 samples across a range of experiments from published studies, encompassing a total of 1868 data points. This data set underwent a normalization process before being randomly segregated into three groups: 70% for training, 15% for testing, and 15% for validation. The training set, constituting the majority of the data, was utilized to adjust model parameters such as weights and biases, ensuring that the model learns the underlying patterns. The testing set was set aside to serve as a benchmark for evaluating the model performance, providing an unbiased assessment of how well the model generalizes to unseen data. The validation set was used to fine-tune the model's hyperparameters, which are crucial for optimizing performance and preventing over-fitting.[46]

2.3. Verification. In this study, to evaluate the effectiveness and validate the performance of both ANN-based models and the MG model, three principal statistical measures are used: R^2, RMSE, and MAE, as detailed in eqs 3−5, respectively. RMSE is a crucial gauge of the models' precision in predicting responses. This measure is particularly significant when the primary goal is prediction accuracy, as it quantifies the extent to which the experimental data points deviate from the predicted values. A lower RMSE value indicates a more accurate model fit, demonstrating close alignment between the predicted and actual data.

R^2 is instrumental in assessing the models' fit. It quantifies the proportion of variance in the observed data that the model accounts for, effectively evaluating how well the data points align with the fitted regression line. A higher R^2 value—closer to 1—indicates that a larger portion of the variance in the observed data is captured by the model, suggesting a more precise depiction of the data through the model's predictions.

Additionally, MAE is employed to measure the average magnitude of the errors in a set of predictions without considering their direction. This metric quantifies the average absolute difference between the predicted values and actual values, offering a clear representation of the prediction error magnitude. A lower MAE value indicates a closer fit of the model to the observed data, enhancing the understanding of the model's predictive performance. Thus, alongside RMSE and R^2, MAE completes a comprehensive statistical framework for assessing model accuracy and fit.

$$R^2 = 1 - \frac{\sum_{i=1}^{N} (\mathrm{Exp}_i - \mathrm{Pre}_i)^2}{\sum_{i=1}^{N} (\mathrm{Exp}_i - \overline{\mathrm{Pre}_i})^2} \tag{3}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum (\mathrm{Exp}_i - \mathrm{Pre}_i)^2}{N}} \tag{4}$$

$$\mathrm{MAE} = \frac{1}{n} \sum_{i=1}^{n} |\mathrm{Exp}_i - \mathrm{Pre}_i| \tag{5}$$

In the equations, Exp_i is the CBY value obtained experimentally; Pre_i is the CBY value calculated from the MG and ANN models; $\overline{\mathrm{Pre}_i}$ is the mean value of predicted data; and N is the number of data points.

3. RESULTS AND DISCUSSION

This section encompasses four integral parts, each examining critical aspects of the predictive models developed in this study. Initially, the results of the MG model are detailed, emphasizing the enhancement of the model's predictive performance. Following this, the outcomes of the ANN-based model are discussed, providing insights into its application and accuracy. A comparative analysis between the ANN and MG models is then conducted to evaluate their relative efficacies. Finally, the significance of the model input parameters is clarified, highlighting their influence on the predictive results. This comprehensive examination not only highlights the unique advantages of each model but also places their performance in the wider context of biogas production prediction.

3.1. Results of the MG Model. The examination of the MG model, as presented in Table 2, shows a detailed evaluation across six case studies involving 39 experiments focused on the influence of microwave pretreatment on AD processes. Each case study presents distinct behaviors in biogas production, with variations evident in the model's fit and predictive accuracies, as evidenced by the differing R^2, RMSE, and MAE values.

The R^2 values, which are essential for assessing the model fit, exhibit significant variation across the case studies. For instance, high R^2 values in case II (0.96) and cases III and VI (both 0.97) suggest that the MG model effectively captures the variability in the experimental outcomes in these scenarios. Conversely, lower R^2 values in case IV (0.83) and case V (0.87) indicate a poorer fit, which may be attributed to the complexity and variability of the biogas production process under different sludge conditions that the model does not adequately represent.

Moreover, the RMSE and MAE values further underline the model's varying performance. Lower values in case II reflect higher accuracy and precision in prediction, while higher values in cases IV and V suggest significant deviations between observed and predicted data, indicating potential deficiencies in the model's capacity to adapt to the complexities introduced by various pretreatment conditions.

The inherent limitation of the MG model, with its reliance on only three parameters (K_1, K_2, and K_3), restricts its flexibility to fully characterize the impacts of different microwave pretreatment conditions on the AD process. This simplistic parametrization may not capture more complex biological and chemical interactions, such as microbial inhibition or synergistic effects, which could be critical in the context of pretreatment variations.

This analysis underscores the necessity of augmenting the MG model or adopting more sophisticated modeling approaches that integrate additional variables and interaction terms. Enhancements to the model could significantly improve its sensitivity to changes in operational conditions and substrate characteristics, thereby providing a more accurate and reliable tool for predicting biogas production in AD processes. ANN-based model, with its capability to adapt to complex, nonlinear relationships by adjusting input data, could effectively enhance the reflection of pretreatment effects on the AD process. By incorporating a broader range of experimental data that reflect diverse operational conditions, the limitations of the current MG model can be addressed. These improvements may facilitate a more comprehensive understanding of

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the dynamics involved in biogas production under varied pretreatment conditions, leveraging the strengths of ANN to dynamically adjust to the intricate dependencies and interactions inherent in AD systems.

3.2. Results of ANN-Based Models. In this section, three training methods, ANN, DFFBP, and DCFBP - are employed to predict CBY. The ANN model, which contains only one hidden layer, is influenced by the number of neurons in this layer. Generally, a higher number of neurons improves the model's performance in fitting data.[47] However, it is important to note that an excessive number of neurons can lead to overfitting. Table 3 demonstrates how the number of neurons

Table 3. Variation in the Number of Neurons in the Hidden Layer of the ANN Model

test no.	hidden neurons no.	$R_{Training}$	$R_{Validation}$	R_{Test}	R_{All}	MAE
1	7	0.9795	0.9823	0.8271	0.9633	19.84
2	8	0.989	0.9696	0.9258	0.9614	13.85
3	9	0.9883	0.9849	0.958	0.9807	13.56
4	10	0.9999	0.9249	0.6977	0.8854	27.37
5	11	0.983	0.5703	0.7188	0.8788	33.54
6	12	0.9026	0.7639	0.8141	0.8571	25.03

in the hidden layer varies from 7 to 12. Through adjustments in $R_{Training}$, $R_{Validation}$, R_{Test}, R_{All}, and MAE, the optimal ANN model was determined to have 9 neurons in the hidden layer. The performance indices for this model are as follows: $R_{Training}$ = 0.9883, $R_{Validation}$ = 0.9849, R_{Test} = 0.958, R_{All} = 0.9807, and MAE = 13.56.

Based on the optimal ANN model with 9 neurons in the hidden layer, the DFFBP model was developed. Table 4

Table 4. Variation in the Number of Hidden Layers of the Deep Feedforward Backpropagation Model

test no.	hidden layers no.	$R_{Training}$	$R_{Validation}$	R_{Test}	R_{All}	MAE
1	2	0.9986	0.983	0.8697	0.9752	8.94
2	3	0.9742	0.9934	0.8428	0.9493	11.96
3	4	0.9813	0.9747	0.8562	0.9523	17.7
4	5	0.9947	0.9969	0.975	0.9913	13.56
5	6	0.9997	0.9852	0.9802	0.9873	6.52
6	7	0.9949	0.9876	0.6329	0.8793	29.52

displays the variation in the number of hidden layers, each containing 9 neurons, ranging from 2 to 7 layers. Through adjustments in $R_{Training}$, $R_{Validation}$, R_{Test}, R_{All}, and MAE, the optimal DFFBP model was determined to have 5 hidden layers, with each layer containing 9 neurons. The performance indices for this model are as follows: $R_{Training}$ = 0.9947, $R_{Validation}$ = 0.9969, R_{Test} = 0.975, R_{All} = 0.9913, and MAE = 13.56. Figure 6 illustrates the regression parameters for the optimal DFFBP model with 5 hidden layers.

Employing the DCFBP model, which is distinguished from the DFFBP model by its incorporation of dynamic continuous feedback processes, allows for real-time adjustment of neuron weights based on error correction feedback, leading to more adaptive learning capabilities.[44] This approach enables the DCFBP model to maintain a continuous flow of updates that potentially enhances predictive accuracy. Similar to the previous studies, this model was structured with 9 neurons per hidden layer but explored variations in the architecture from 2 to 7 hidden layers, as shown in Table 5. Optimizing the configuration involved systematic adjustments in $R_{Training}$, $R_{Validation}$, R_{Test}, R_{All}, and MAE metrics. The most effective structure was found to include 4 hidden layers, significantly refining performance outcomes. Specifically, the DCFBP model yielded $R_{Training}$ at 0.9989, $R_{Validation}$ at 0.9882, R_{Test} at 0.9697, R_{All} at 0.9946, and achieved a lower MAE of 0.34. Figure 7 provides a detailed visualization of the regression parameters for this optimal model configuration, showcasing the DCFBP's superior ability to dynamically integrate and process feedback, which is critical for handling complex and evolving data sets more efficiently than the static approach of the DFFBP model.

After optimization of the number of neurons and hidden layers, the most effective model for predicting CBY among ANN, DCFBP, and DFFBP is identified as DCFBP. Whether evaluated by the R^2 or the MAE, DCFBP consistently outperforms the other models. This superior performance can be attributed to DCFBP's unique architectural framework, which integrates multiple cascaded layers and forward–backward information flow that enhances model depth and learning capacity.

DCFBP's design allows for a more nuanced handling of complex patterns and interactions within the data, significantly improving predictive accuracy. The cascaded architecture facilitates deeper learning by enabling the network to refine its understanding of data features at multiple levels, an advantage not typically found in simpler ANN models or DFFBP configurations. Moreover, DCFBP benefits from sophisticated training algorithms that optimize layer-specific parameters, minimizing error throughout the network and increasing the stability of the predictions. This combination of depth and precision makes the DCFBP model particularly effective in fields such as biogas yield forecasting, where accuracy is paramount.

3.3. Comparison of ANN and MG Models. As the DCFBP model demonstrated the best performance among the three evaluated ANN models, a comparative analysis was conducted to evaluate the predictive accuracy and model fitness of the MG and DCFBP models, as depicted in Figure 8. The experimentally obtained CBY values are represented by circles, while the predictions from the DCFBP and MG models are indicated by crosses and solid lines, respectively. The analysis revealed that both models closely align with the experimental CBY trajectories. However, the DCFBP model demonstrated superior predictive accuracy when compared with the MG model, suggesting enhanced reliability and precision in capturing the dynamics of biogas production over the digestion period.

Figure 8 indicates that both models effectively correspond to the experimental data. However, when combined with results from Tables 2 and 5, it suggests that the DCFBP model is more precise for this application and serves as a viable alternative to kinetic modeling. The performance of DCFBP is notably more stable than that of the MG model, regardless of the type of the sludge substrate and the conditions of pretreatment. This higher accuracy may stem from the ANN models' ability to discern complex, nonlinear relationships between input and output data without relying on prior knowledge or intricate mathematical equations.[48] The ANN models establish connections among input, hidden, and output layers, potentially improving its accuracy. Moreover, the DCFBP model excels in predicting CBY in one integrated

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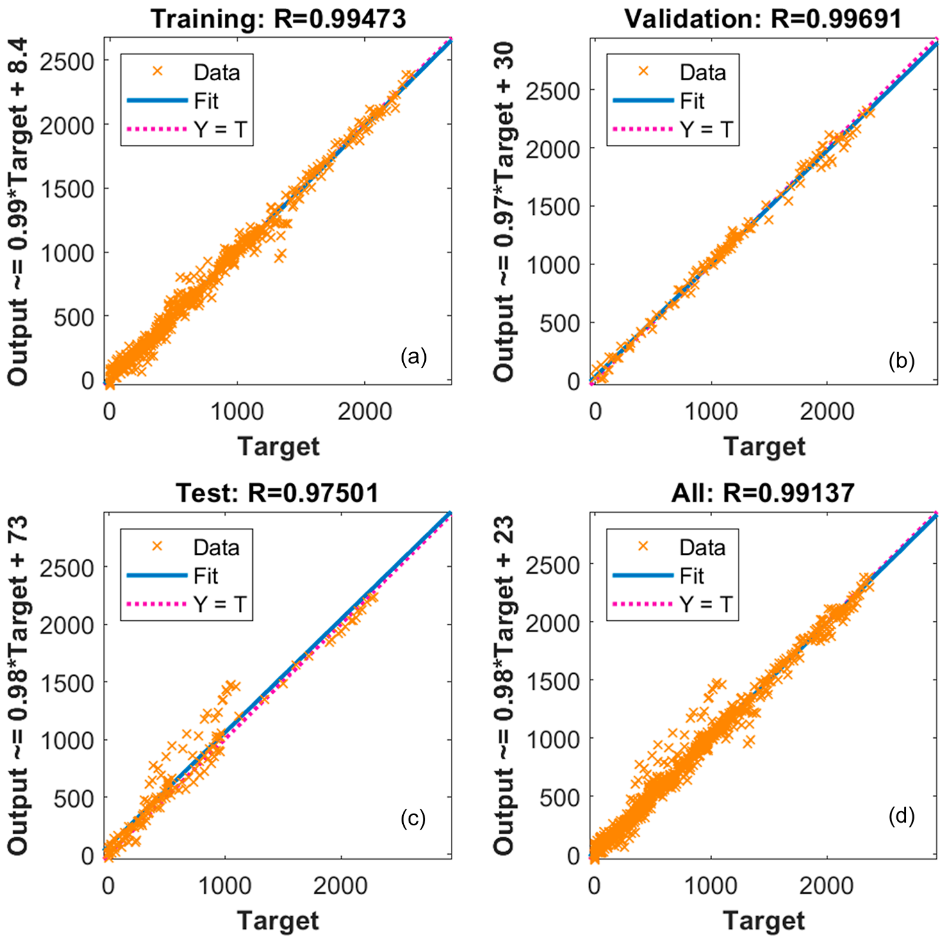

Figure 6. Results of the deep feed forward backpropagation model (a) training; (b) validation; (c) test; (d) all.

Table 5. Variation in the Number of Hidden Layers of the Deep Cascade Forward Backpropagation Model

test no.	hidden layers no.	$R_{Training}$	$R_{Validation}$	R_{Test}	R_{All}	MAE
1	2	0.9865	0.7364	0.9776	0.9328	18.81
2	3	0.9586	0.7526	0.9693	0.9374	20.96
3	4	0.9989	0.9882	0.9697	0.9946	0.34
4	5	0.9774	0.9497	0.8409	0.9597	9.58
5	6	0.8327	0.855	0.5608	0.7495	86.4
6	7	0.8972	0.6571	0.6218	0.7254	39.71

process, in contrast to the MG model, which necessitates separate development and numerous iterations for each type of substrate mixture, leading to a more time-intensive process. The results from computational analyses underscore the strength and efficiency of the ANN approach. This method stands out, particularly for its adeptness in managing complex, high-dimensional data sets, attributed to its rapid processing, ability to generalize, and superior learning capabilities. As such, it presents itself as an advantageous alternative to conventional kinetic models.

3.4. Relative Importance of Model Input Parameters. Figure 9 presents a heatmap visualization that assesses the relative importance and influence of various input parameters across the neurons in the final hidden layer of the DCFBP model. This heatmap is color-coded to illustrate both the magnitude and direction of each parameter's influence on the model's output. The parameters analyzed include microwave power level (1), sample volume (2), temperature reached after microwave processing (3), VS/TS (4), SCOD/TCOD (5), and DT (6). These inputs are crucial for assessing the efficiency and optimization of treatment systems that incorporate microwave processing. The color gradation, ranging from red to blue, signifies the varying degrees of each parameter's influence, with red denoting a lesser influence and blue indicating a greater impact. This detailed visualization captured in the heatmap offers valuable insights into how each parameter potentially contributes to the overall system performance, thereby facilitating targeted adjustments in-process controls to improve both efficiency and efficacy.

This visual analysis is quantitatively supported by the average and median weights presented in Table 6, which further elucidates the role of each parameter. Notably, "VS/TS" (4) and "SCOD/TCOD" (5) consistently display a pivotal influence across different neurons, underscoring their roles in reflecting chemical composition changes during the microwave processing (MP) phase. These parameters not only show the highest positive average and median weights (average: 0.31016 for VS/TS and 0.33225 for SCOD/TCOD) but are also visually highlighted on the heatmap, indicating their substantial impact on the model's output.

Additionally, temperature reached after MP' (3) and "DT" (DT, 6) are also significant, with their effects on the prediction results being critical, albeit varied. While "temperature after MP" shows a relatively neutral average weight (0.0177), its negative median weight (−0.31056) points to its complex role

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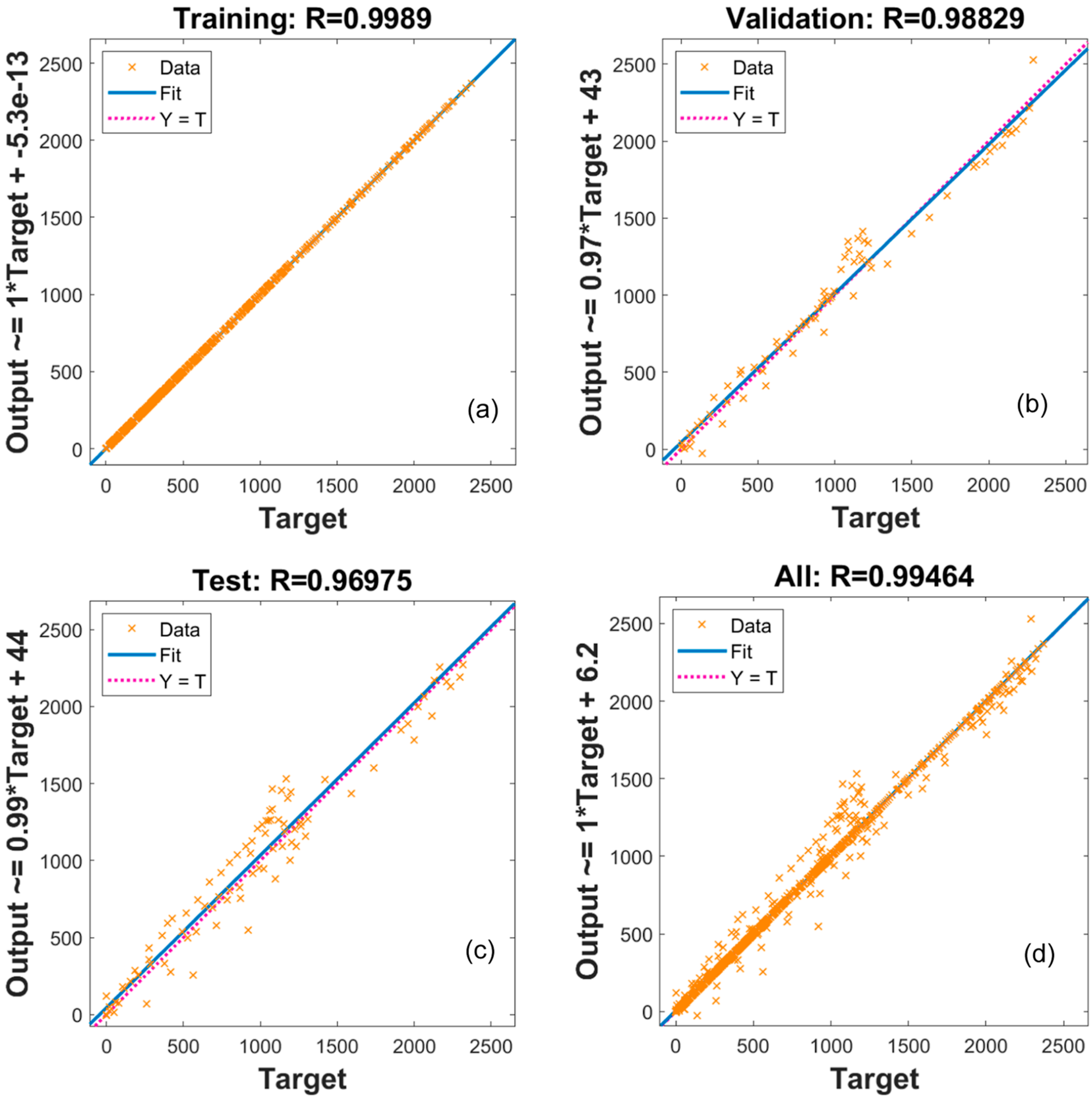

Figure 7. Results of the deep cascade forward backpropagation model (a) training; (b) validation; (c) test; and (d) all.

under varying operational conditions. "DT" emerges as a consistently critical but limiting factor, reflected by the most negative influence across both average and median weights (average: −0.46601, median: −0.35695). As discussed in Section 2.1, temperature variations indicate the conditions of the MP process, directly correlating with "digestion time" to the final biogas yield, aligning well with experimental observations. Although higher microwave power levels can yield more biogas at the same temperature, as noted in Section 3.1, their weight does not reflect this influence directly. Instead, changes in VS/TS and SCOD/TCOD encapsulate this effect, indicating that while the microwave power level is an indirect factor, the model comprehensively accounts for its effects through these more prominently weighted parameters.

This integrated analysis highlights the integral roles of "VS/TS" and "SCOD/TCOD" in modeling the MP process and underscores the importance of "temperature after MP" and "DT" in accurately predicting biogas yield, providing a nuanced understanding of how each parameter contributes to system performance and efficiency. This facilitates targeted improvements in process controls and can guide further research and development efforts.

3.5. Practical Applications, Research Significance, and Future Work. The primary advantage of the DCFBP model is its enhanced predictive accuracy, as it demonstrated higher R^2 values (0.9946) and lower MAE (0.34) scores across various case studies compared to those of the MG model. This indicates that the DCFBP model can more reliably predict CBY in AD processes, allowing for better operational decisions and optimizing feedstock inputs and process parameters to maximize biogas production, leading to significant cost savings and improved efficiency in biogas facilities.[23] Tested on 39

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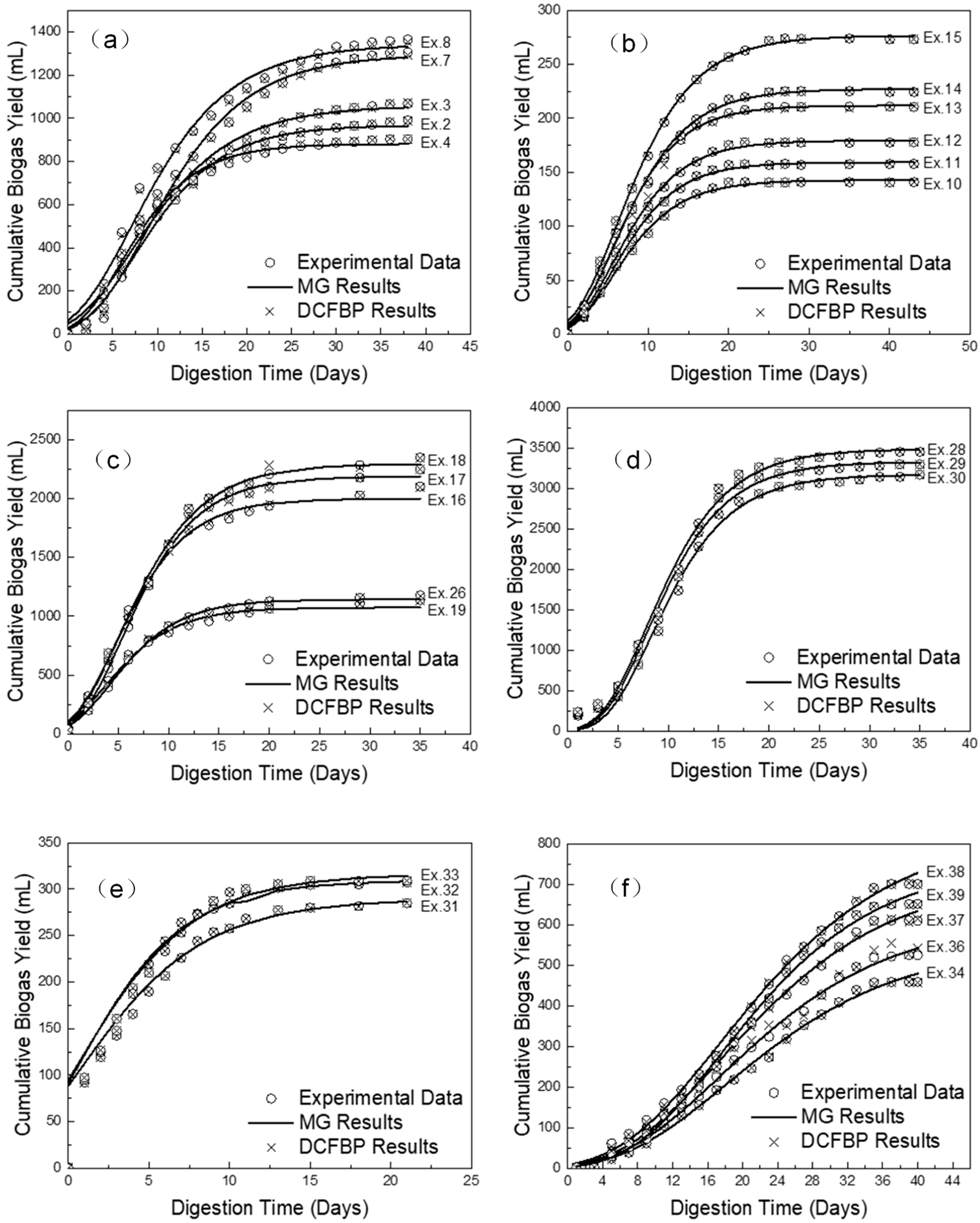

Figure 8. Results of the optimized models for the different experimental cases, (a) case I, (b) case II, (c) case III, (d) case IV, (e) case V, and (f) case VI.

different experimental cases with varying sludge substrates and pretreatment conditions, the model showcased its robustness and versatility, making it a valuable tool for industry practitioners dealing with diverse organic wastes. Its adaptability allows it can handle different types of sludge and operating conditions, providing reliable predictions across different settings under microwave pretreatment. The robustness of the DCFBP model suggests scalability from laboratory settings to commercial AD operations, which is crucial for real-world applications. By providing accurate predictions for biogas yield, the model can help facilities optimize their operations, leading to increased biogas production and more efficient waste-to-energy conversion processes.[49] Its ability to generalize across different data sets and conditions makes it a practical tool for enhancing biogas production on a larger scale. Efficient biogas production contributes to environmental

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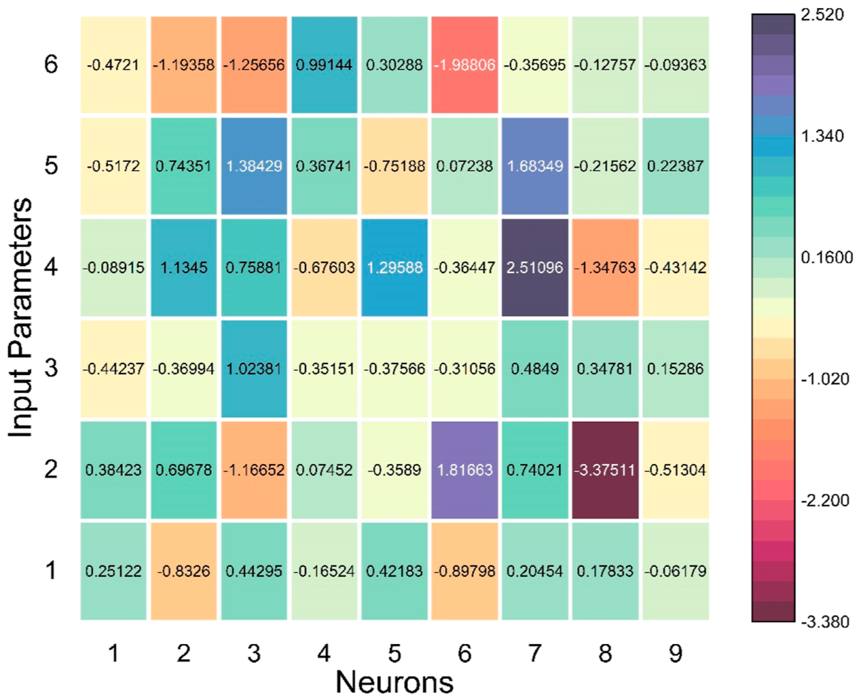

Figure 9. Importance evaluation of input parameters with neurons [(1). Microwave power level; (2). Sample volume; (3). Temperature reached after MP; (4). VS/TS; (5). SCOD/TCOD; and (6). DT].

Table 6. Average and Median Weights of Input Parameters in the DCFBP Model

	input 1 (microwave power level)	input 2 (sample volume)	input 3 (temperature reached after MP)	input 4 (VS/TS)	input 5 (SCOD/TCOD)	input 6 (DT)
average weights	−0.05097	−0.18902	0.0177	0.31016	0.33225	−0.46601
median weights	0.17833	0.07452	−0.31056	−0.08915	0.22387	−0.35695

sustainability by reducing greenhouse gas emissions and promoting the use of renewable energy sources. By improving the efficiency of biogas production, the DCFBP model supports these environmental goals, optimizing the AD process and maximizing biogas yields from organic waste, contributing to a more sustainable and environmentally friendly energy production method. The findings of this study address the primary research questions by demonstrating that the DCFBP model significantly improves the accuracy of biogas yield predictions in AD processes, capturing complex nonlinear relationships in the data more effectively than traditional kinetic models. The practical implications discussed highlight the model's potential impact on the AD industry, providing a comprehensive answer to the research questions and setting a foundation for future research.

Future research should focus on expanding the application of the DCFBP model to a broader range of real-world data sets, including sludge from different regions and industries. This will help validate the model's generalizability and practical utility across various contexts. Additionally, integrating more advanced machine learning techniques and exploring hybrid models could further enhance the predictive accuracy and adaptability. Exploring the impact of different pretreatment methods and operational conditions on biogas yield predictions will provide deeper insights into optimizing AD processes. Collaboration with industry partners to implement the model in large-scale AD facilities could yield valuable data and feedback, facilitating the continuous improvement of the model. Lastly, assessing the economic and environmental benefits of using the DCFBP model in AD processes can help quantify its value proposition and support its adoption in the industry. By addressing these future directions, research can significantly contribute to the advancement of AD technology and sustainable energy production.

4. CONCLUSIONS

This comprehensive study successfully merges traditional kinetic models with advanced ANN models and microwave processing to enhance biogas production predictions in the AD process. By focusing on microwave pretreatment, the research aimed to enhance the efficiency and yield of biogas production from various organic wastes. The developed models—ANN-FFBP, DFFBP, and DCFBP—demonstrated superior predictive capabilities over traditional models, particularly the DCFBP model, which achieved the highest correlation coefficient (0.9946). A critical aspect of this research was the analysis of the relative importance of model input parameters, such as VS/TS, SCOD/TCOD, post-MP temperature, and DT. These parameters proved essential in assessing and optimizing the process efficiency. This study not only highlights the efficacy of ANN models in delivering user-friendly and efficient prediction methods but also underscores the importance of specific process parameters in enhancing the gas yield of AD. The insights gained from this research facilitate accurate forecasting and optimization of the AD process under various conditions, aiding in scale-up and

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process improvement. Future research should further explore the influence of additional variables and extend the model's application to a wider range of data sets and conditions, thereby contributing to the field of sustainable energy and biogas production.

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Notes

The authors declare no competing financial interest.

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