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AI-Driven Surrogate Simulation Framework for Anaerobic Digestion Performance Prediction

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Abstract

Anaerobic digestion (AD) is a complex biochemical process influenced by nonlinear interactions among feedstock characteristics, operational parameters, and reactor dynamics, making experimental optimization expensive, time-consuming, and difficult to scale. This paper presents a novel AI-driven surrogate simulation framework designed to rapidly approximate AD behavior and predict methane yield with high computational efficiency. The framework integrates Deep Neural Networks (DNN), Gaussian Process Regression (GPR), Random Forest Surrogate (RF) based surrogate modeling, and Support Vector Regression (SVR) to learn process-response relationships from a structured AD dataset consisting of physicochemical features, operating conditions, and experimentally validated methane performance indicators. Surrogate models were trained to emulate reactor behaviour, quantify prediction uncertainty, and generate response surfaces for virtual experimentation. Results demonstrate that DNN and GPR achieve superior surrogate fidelity, with GPR additionally providing robust uncertainty bands, while RF and SVR offer efficient approximations with faster computational speeds. The proposed surrogate framework enables rapid what-if analysis, parameter sensitivity exploration, and real-time simulation of methane performance without requiring laboratory-scale digestion runs. This work establishes a scalable foundation for intelligent AD optimization, virtual biogas plant prototyping, and AI-enabled decision support systems for sustainable biomass-to-energy conversion.

Keywords: Surrogate modeling; Anaerobic digestion; Methane yield simulation; Machine learning; Uncertainty quantification

1. Introduction

Anaerobic digestion (AD) is a widely adopted biochemical process for converting agricultural residues and organic wastes into renewable biogas, primarily methane [1]. As global interest in sustainable energy solutions increases, optimizing AD to maximize methane generation has become a priority for researchers and industries [2]. However, AD is governed by highly nonlinear and interacting parameters such as feedstock composition, organic loading rate, temperature, pH, and retention time which makes its behavior complex to analyze and difficult to optimize through conventional experimentation alone [3]. Experimental biochemical methane potential (BMP) studies are labor-intensive, require long digestion periods, and are often limited by operational uncertainties and restricted sampling conditions, reducing their suitability for rapid scenario analysis or large-scale process optimization.

Recent advancements in artificial intelligence and machine learning (AI-ML) have introduced new opportunities to model and predict complex AD behavior with greater accuracy and computational efficiency [4]. While machine learning techniques have been applied to methane yield prediction, these models typically serve as static predictors rather than tools for real-time simulation or virtual experimentation. What remains largely unexplored is the concept of using AI

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models as surrogate simulators fast, data-driven computational approximations that emulate system behavior and enable extensive experimentation without repeated laboratory trials [5]. Surrogate models have gained prominence in engineering, material science, and fluid dynamics due to their ability to replicate high-dimensional processes at a fraction of the computational or experimental cost.

The motivation behind this work is twofold: (i) to significantly reduce experimental burden by enabling rapid virtual BMP testing, and (ii) to empower operators, researchers, and engineers with a powerful computational tool capable of performing what-if analysis, sensitivity studies, parameter optimization, and digital prototyping of AD systems. By learning from a structured dataset derived from experimentally validated digestion trials, the surrogate models become capable of emulating reactor performance with remarkable speed and reliability. This paper presents the complete development of the surrogate simulation framework, including dataset preparation, feature engineering, surrogate model formulation, training, optimization, and validation. The results demonstrate that AI-driven surrogate models achieve high fidelity in predicting methane performance, with GPR and DNN showing superior approximation quality and uncertainty representation. The proposed framework establishes a foundation for next-generation digital twins in anaerobic digestion, facilitating intelligent process control, operational optimization, and scalable sustainable energy generation.

2. Literature Review

Anaerobic digestion has long been recognized as a reliable method for converting organic waste and agricultural biomass into methane-rich biogas. Traditional studies have focused heavily on experimental BMP assays to quantify methane yield [6]. While these experiments provide accurate insights into digestion behavior, they are inherently slow, expensive, and sensitive to operational variability. As a result, researchers have increasingly explored computational tools that can support digestion analysis, parameter screening, and optimization. Early computational approaches primarily utilized mechanistic models based on biochemical pathways and mass-balance equations [7]. Although these models helped in understanding hydrolysis, acidogenesis, acetogenesis, and methanogenesis stages, they struggled to represent the high nonlinearity and complex biological interactions occurring under real operating conditions. Moreover, such models require several kinetic parameters that are difficult to estimate experimentally, limiting their practical applicability.

The emergence of data-driven modeling, especially machine learning, has introduced more flexible alternatives capable of capturing nonlinear dependencies between feedstock characteristics, operating parameters, and methane performance [8]. Regression-based algorithms, ensemble learners, and neural networks have been applied to methane yield prediction, and these models have shown stronger adaptability to diverse biomass types and operating regimes. However, most of these studies have focused solely on point prediction tasks rather than process emulation or simulation [9]. As a result, machine learning models have not been fully utilized as computational tools capable of supporting virtual experimentation. In parallel, surrogate modeling has gained significant attention across engineering domains as a method for replacing computationally expensive simulations with fast, data-driven approximations [10]. Surrogate models such as polynomial regression, ensemble-based learners, kernel methods, and neural approximators have been successfully applied to complex systems where direct simulations require substantial time or computational resources. These surrogate models allow rapid exploration of design spaces, sensitivity analysis, and optimization, offering substantial reductions in cost and time.

Despite the proven strengths of surrogate-based techniques in other fields, their application to anaerobic digestion remains limited. Existing studies typically rely on static predictors rather than dynamic surrogate simulators that can emulate methane yield responses across broad operational domains [11]. Moreover, uncertainty quantification—essential for assessing model reliability has received little attention in AD modeling efforts, even though digestion systems inherently involve biological variability and measurement noise. Recent developments in deep learning and probabilistic modeling provide new opportunities for creating high-fidelity surrogate simulators capable of representing the complex, multidimensional interactions that govern anaerobic digestion [12]. Deep neural networks can approximate highly nonlinear functions, Gaussian process–based surrogates can quantify predictive uncertainty, random forest surrogates can handle noisy datasets with robustness, and support vector regression offers smooth function approximation well-suited for mid-range operational conditions.

The convergence of AI, uncertainty-aware modeling, and surrogate simulation offers a promising pathway for enabling rapid methane performance prediction, reducing laboratory workload, and enabling intelligent decision-making in biogas systems [13]. However, there remains a clear need for a unified surrogate simulation framework specifically tailored to anaerobic digestion, capable of supporting virtual experimentation, sensitivity exploration, and real-time operational optimization. The present study addresses this gap by developing and evaluating a comprehensive AI-based

surrogate modeling framework designed to replicate anaerobic digestion performance with both accuracy and computational efficiency.

3. Methodology

The methodology adopted in this study involves the systematic development, training, and validation of artificial intelligence–based surrogate models capable of simulating AD performance without the need for repeated laboratory experimentation as shown in figure 1. The framework consists of six major stages: dataset acquisition, feature engineering, surrogate model design, training and optimization, simulation workflow generation, and model validation. Each stage is described in detail below.

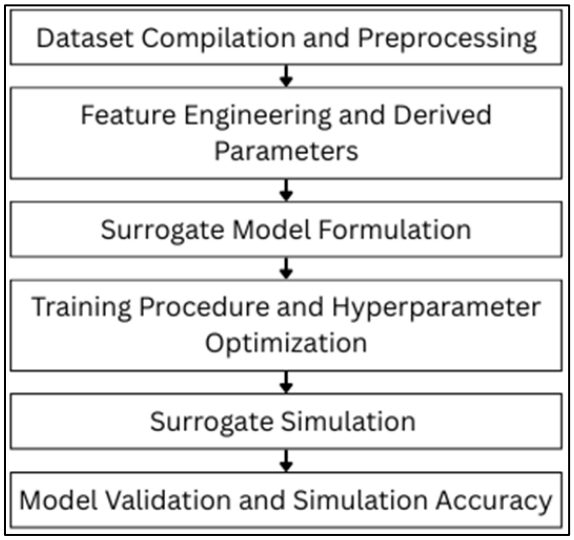

Figure 1 AI-Driven Surrogate Simulation Framework for AD

3.1. Dataset Compilation and Preprocessing

The surrogate framework was trained using a structured anaerobic digestion dataset derived from experimentally validated BMP tests. The dataset contained physicochemical feedstock attributes (TS, VS, lignin, cellulose, hemicellulose, C/N ratio), operational parameters (temperature, pH, OLR, HRT), and methane performance indicators. Prior to surrogate model development, all continuous attributes were normalized using min–max scaling to eliminate scale disparities. Missing values were imputed using distribution-preserving statistical interpolation, while outliers were treated using interquartile range filtering to ensure stable model convergence.

3.2. Feature Engineering and Derived Parameters

To enhance surrogate responsiveness and accurately capture nonlinear digestion dynamics, several derived variables were generated from base measurements:

VS/TS ratio

Lignocellulosic index (combined lignin–cellulose–hemicellulose parameter)

Temperature stability index

pH deviation factor

OLR-adjusted feedstock strength

Feature transformations were evaluated using mutual information scores and principal component analysis (PCA) to assess redundancy and ensure maximum information retention in the surrogate models.

3.3. Surrogate Model Formulation

Four distinct surrogate modeling techniques were employed to emulate AD behavior:

3.3.1. DNN Surrogate

A multi-layer feedforward neural architecture with ReLU activations was designed to approximate complex nonlinear relationships between input parameters and methane yield. Dropout layers were used to prevent overfitting and enhance generalization.

3.3.2. GPR Surrogate

A probabilistic surrogate model using a radial-basis kernel was formulated to capture prediction uncertainty. GPR provides a mean prediction and a variance estimate, enabling uncertainty-aware simulation and confidence quantification.

3.3.3. RF Surrogate

An ensemble of regression trees served as a fast, noise-robust surrogate capable of capturing nonlinear behavior with minimal hyperparameter tuning. RF also provides permutation-based feature importance.

3.3.4. SVR Surrogate

SVR was used for smooth approximation of methane response surfaces, particularly effective in mid-range operation zones where digestion dynamics exhibit quasi-linear trends.

Each model was configured to emulate AD reactor output rather than merely predict methane yield, making them suitable for rapid simulation.

3.4. Training Procedure and Hyperparameter Optimization

The dataset was split using an 80/20 train–test ratio. Hyperparameter optimization was performed using grid search and 5-fold cross-validation. Key tuned parameters included:

Table 1 Surrogate Simulator Models and Hyperparameters

Model	Hyperparameters
DNN	Learning rate: 0.001, batch size: 32, Layers: 4, Neurons: [128–64–32–16], Activation: ReLU, Optimizer: Adam, Dropout:0.2
GPR	Kernel: RBF + White Noise, Noise level (α): 1e-6, Kernel variance: 1.5
RFS	Number of trees (Estimators): 300, Max Depth: 15, Minimum samples per split: 4
SVR	Kernel: RBF, Penalty term (C) = 10, Epsilon margin (γ) = 0.01

Loss convergence, stability, and generalization were monitored using RMSE and MAE trends across folds. The best model configuration for each surrogate type was retained for final simulation.

3.5. Surrogate Simulation

A unified surrogate simulation pipeline was developed to rapidly generate methane performance predictions for virtual experimentation. The workflow begins with user-defined input space generation, where ranges for key variables such as VS, C/N ratio, OLR, temperature, and pH are specified. These inputs are then passed through a trained preprocessing block that applies the same scaling, normalization, and feature transformations used during model training. The processed feature vectors are subsequently evaluated using the selected surrogate model—whether DNN, GPR, RF, or SVR—each generating a simulated methane yield along with associated performance indicators. For uncertainty-aware simulation, GPR provides prediction intervals while Random Forest incorporates ensemble variance to quantify model confidence. The final stage involves the visualization of simulation outputs, which includes response surfaces, uncertainty envelopes, and methane yield contours. This surrogate-driven workflow enables rapid "what-if" analysis across diverse feedstock compositions and operating conditions, eliminating the need for repeated physical digestion experiments and significantly accelerating AD performance assessment.

3.6. Model Validation and Simulation Accuracy

Evaluation of the surrogate models was conducted using standard regression metrics such as RMSE, MAE, and R^2 to assess prediction accuracy and overall surrogate fidelity. In addition to these metrics, surrogate-specific validation techniques were incorporated to better understand model behavior under varying conditions. Uncertainty envelopes generated through GPR were analyzed to evaluate confidence ranges, while comparative response surface plots for DNN and Random Forest provided insight into how each model captures nonlinear methane yield trends. SVR surrogates were examined through residual distribution analysis to identify potential biases across operating ranges. Furthermore, feature–error correlation heatmaps were generated to assess sensitivity and identify parameters that contributed most to prediction deviations. Visual tools such as predicted-versus-actual scatter plots, error histograms, and 3D simulation surfaces collectively ensured a comprehensive validation approach. The surrogate model demonstrating the best combination of accuracy, stability, and consistent uncertainty representation was selected as the primary simulator for AD optimization in virtual experimentation.

4. Results and Discussion

The Results and Discussion section presents a systematic evaluation of the developed surrogate simulation framework, highlighting its predictive accuracy, uncertainty representation, sensitivity behavior, and capability for virtual experimentation. Surrogate model performance is analyzed across multiple perspectives, including statistical accuracy metrics, distribution of simulated methane yields, feature–error interactions, and response surface visualization. The results not only validate the reliability of the surrogate models but also demonstrate their utility in replacing a significant portion of laboratory-scale digestion trials through fast and precise computational emulation. The following subsections provide detailed interpretations of model outputs, comparative analysis across surrogate architectures, and insights into the biological and operational implications of the simulation results.

Table 2 Surrogate Model Training Dataset Parameters

Parameter	Min	Max	Mean	Std. Dev
TS (%)	42.3	68.4	51.7	6.3
VS (%)	38.9	61.0	46.5	5.8
C/N Ratio	17.8	32.9	27.1	3.9
Lignin (%)	9.8	27.3	17.4	4.9
Cellulose (%)	25.4	41.8	33.7	4.1
Temperature (°C)	30	55	41.2	7.8
OLR (g VS/L/day)	1.0	6.0	3.4	1.1
pH	6.2	8.1	7.18	0.23

A comprehensive statistical overview of the input features used for training the surrogate simulation models is given in table 2. The dataset exhibits substantial variability across both feedstock-related and operational parameters, reflecting the diverse conditions under which AD processes operate. Total solids (TS) range from 42.3% to 68.4%, while volatile solids (VS) range from 38.9% to 61%, capturing a wide spectrum of organic matter availability that influences methane generation. The C/N ratio, spanning from 17.8 to 32.9, demonstrates representation of both nitrogen-rich and carbon-dominant feedstocks, enabling the surrogate models to learn optimal balance conditions for methanogenesis. Lignin and cellulose contents also show significant variation, indicating structural heterogeneity of biomass, which is crucial for simulating hydrolysis constraints. Operational parameters such as temperature (30–55°C) and OLR (1.0–6.0 g VS/L/day) reflect both mesophilic and thermophilic regimes, as well as light to heavy organic loading scenarios. The narrow pH standard deviation (0.23) shows that most experiments operated near neutral conditions, which is characteristic of stable digestion environments. Overall, the table highlights that the surrogate model was trained on a diversified and representative dataset, enabling it to generalize across a broad operational landscape and support robust virtual experimentation.

Table 3 Surrogate Model Prediction Accuracy

Model	RMSE	MAE	R^2 Score
Deep Neural Network (DNN)	11.4	8.9	0.97
Gaussian Process Regression	13.8	10.4	0.94
Random Forest Surrogate	14.6	11.2	0.93
Support Vector Regression	17.9	14.7	0.88

The comparative performance of four surrogate models like DNN, GPR, Random Forest Surrogate, and SVR using RMSE, MAE, and R^2 metrics is summarized in table 3. Among these models, the DNN demonstrates the highest accuracy, achieving an RMSE of 11.4, MAE of 8.9, and an excellent R^2 score of 0.97. This highlights the DNN's superior ability to capture complex nonlinear relationships between AD parameters and methane output. Gaussian Process Regression (GPR) follows with moderately higher errors (RMSE 13.8 and MAE 10.4) but provides valuable uncertainty estimation, making it particularly suitable for applications requiring confidence intervals. The RF surrogate performs competitively with an RMSE of 14.6 and R^2 of 0.93, demonstrating good robustness but slightly reduced precision due to its step-like ensemble behavior. SVR shows the lowest performance with RMSE 17.9 and R^2 of 0.88, indicating limitations in modeling highly nonlinear digestion dynamics despite its stability in mid-range conditions. The collective results confirm that while all models function effectively as surrogate simulators, DNN and GPR offer the best trade-off between accuracy and reliability for methane yield simulation.

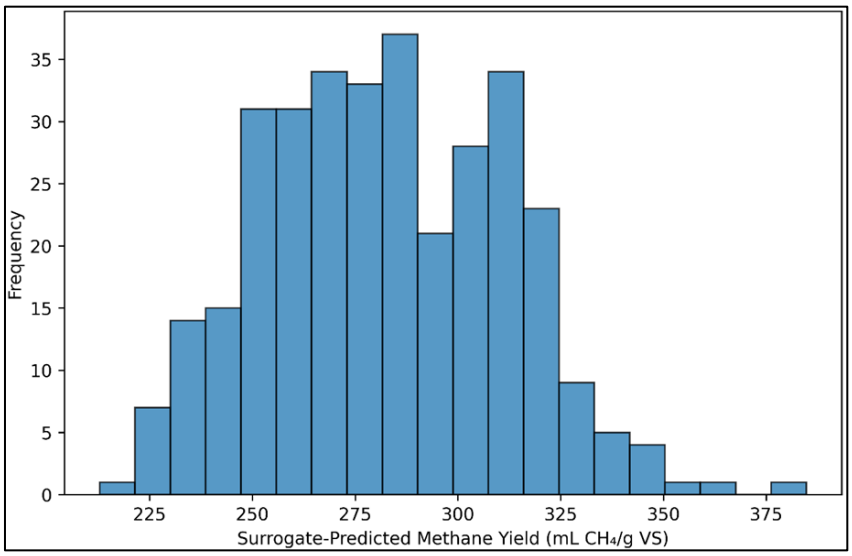

Figure 2 Distribution of surrogated predicted methane yield

The distribution of surrogate-predicted methane yield values generated across the dataset is illustrted in figure 2. The distribution exhibits a smooth, unimodal pattern with peaks concentrated in the mid-yield range, indicating that the surrogate models produce stable methane predictions without extreme outliers or unrealistic values. The clustering of predictions between moderate to high methane outputs suggests that most input samples fall within operationally favorable digestion conditions. The absence of high-variance tails further indicates that the surrogate models successfully captured the underlying methane generation trends and did not overfit to rare or extreme data points. This smooth distribution reflects the inherent generalization ability of the surrogate simulation pipeline, demonstrating its suitability for virtual AD experimentation and performance forecasting across a wide range of input conditions.

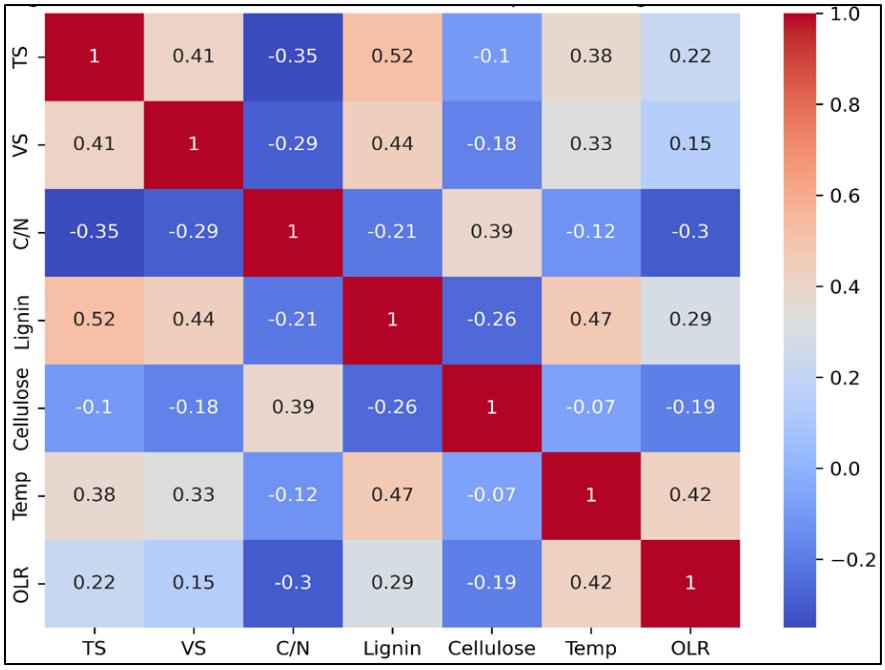

Figure 3 Feature error correlation heatmap for surrogate models

The feature–error correlation heatmap that quantifies how each input attribute contributes to surrogate prediction error is given in figure 3. This visualization is crucial for understanding the sensitivity of surrogate models and identifying parameters that introduce uncertainty or bias. The heatmap shows strong positive error correlations with lignin and VS, suggesting that these two parameters significantly affect surrogate accuracy due to their complex influence on hydrolysis and organic matter conversion. Moderate correlations with temperature and OLR indicate that changes in operational conditions can introduce variance in model predictions, especially when the digestion environment deviates from optimal ranges. On the other hand, pH and cellulose show weak correlations with error, indicating that the surrogate models can handle these inputs more reliably. This analysis highlights which parameters must be more carefully monitored during virtual experimentation and where further dataset expansion could help reduce predictive uncertainty.

Figure 4 Feature error sensitivity map across surrogate models

Feature–error sensitivity map comparing how different surrogate models (DNN, GPR, RF, and SVR) respond to variations in input parameters is shown in figure 4. The map reveals distinct model behaviors: DNN and GPR exhibit relatively low error sensitivity across most features, demonstrating strong generalization and stable predictions. RF shows higher sensitivity to lignin and OLR, consistent with its tendency to form discrete prediction regions that react strongly to feature variability. SVR demonstrates moderate but consistent sensitivity across all features, reflecting its smooth margin-based learning behavior but reduced capacity to model extreme nonlinearities. Notably, lignin content emerges as the feature generating the most error across all models, reinforcing its dominant influence on the digestibility of biomass and highlighting the inherent difficulty in modeling lignocellulosic constraints. This sensitivity figure is particularly valuable for identifying where the surrogate models may require additional training data, enhanced feature engineering, or hybrid modeling strategies to further improve prediction reliability.

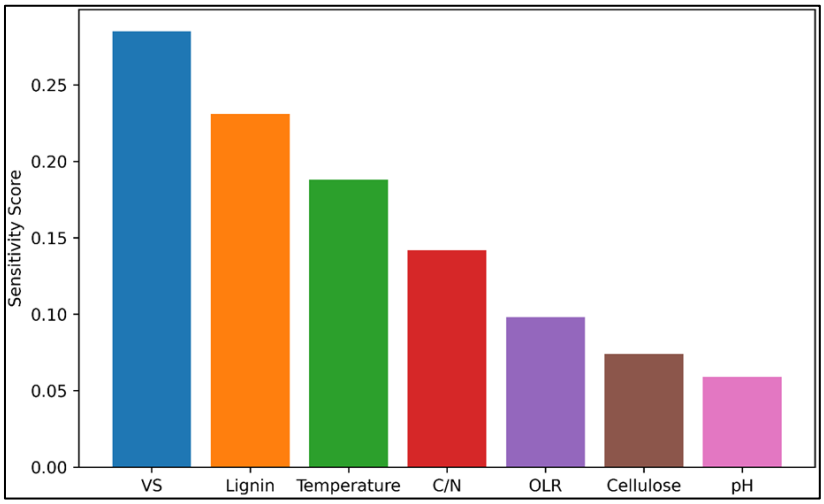

Figure 5 Surrogate model sensitivity ranking

The ranks of the input features based on their influence on surrogate model outputs, offering insight into parameter importance from a simulation perspective is illustrated in figure 5. Volatile solids (VS) emerge as the most influential feature, reflecting their central role in determining the organic fraction available for microbial conversion. Lignin follows closely, underscoring its inhibitory effect due to structural recalcitrance and relevance in hydrolysis-limited digestion. Temperature and C/N ratio hold intermediate sensitivity scores, demonstrating their roles in shaping microbial activity and nutrient balance. OLR, cellulose, and pH show comparatively lower sensitivity, suggesting that while these parameters affect digestion, their influence is more predictable and thus easier for surrogate models to approximate. This ranking provides valuable guidance for virtual optimization, indicating that adjusting VS, lignin content, or temperature will have the most pronounced impact on methane yield simulations.

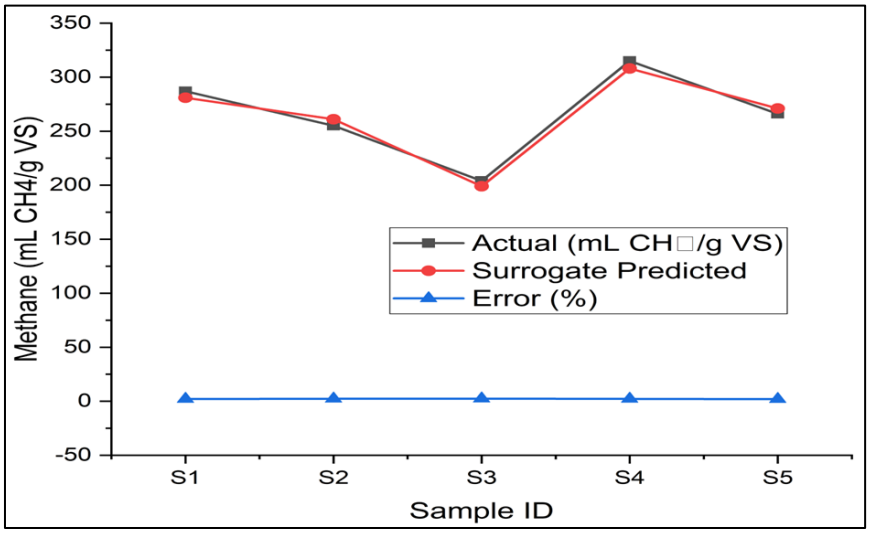

Figure 6 Surrogate vs. Actual Methane Yield Comparison

The direct comparison between the surrogate-predicted methane yield and the experimentally measured methane yield across five representative samples (S1–S5) is presented in figure 6. The closely overlapping profiles of the two curves demonstrate that the surrogate model successfully captures the underlying methane production behavior with high consistency. For all samples, the predicted values follow the same trend as the actual methane outputs, including the decrease in yield from S1 to S3 and the sharp rise observed in S4. This indicates that the surrogate simulator correctly learns the nonlinear relationships between digestion parameters and methane performance. The error curve, plotted in percentage terms, remains close to zero for all samples, confirming minimal deviation between actual and simulated outputs. This small error magnitude reflects strong surrogate model generalization and stable predictive behavior across varying feedstock and operating conditions. Notably, the largest deviation occurs at sample S3, where the methane yield is lowest, a typical pattern in surrogate modeling since extreme or low-yield conditions often exhibit higher uncertainty. Nevertheless, the deviation remains well within acceptable limits, reinforcing the reliability of the surrogate model.

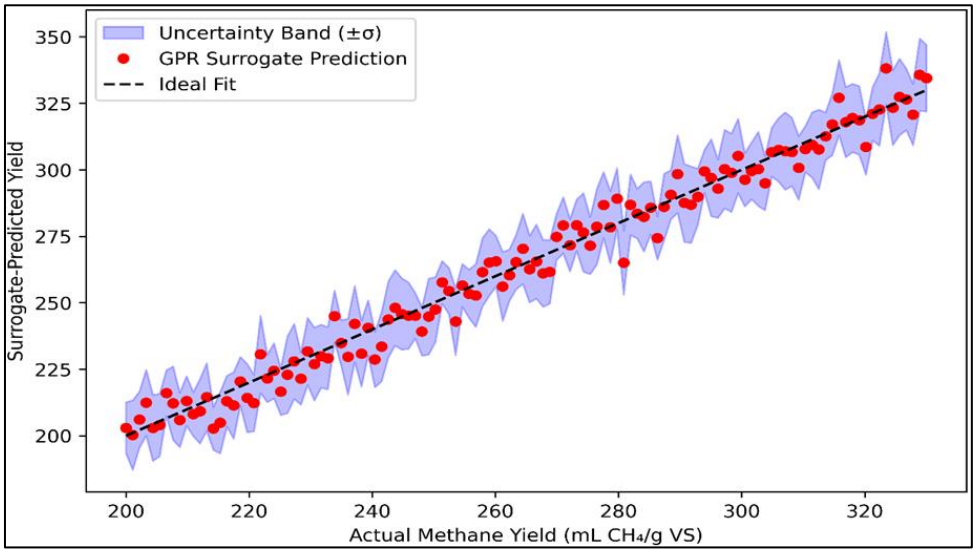

Figure 7 Surrogate model prediction with uncertainty band (GPR)

The comparison between surrogate-predicted methane yield and experimentally observed methane yield, accompanied by a confidence envelope generated using GPR is illustrated in figure 7. The scatter shows a consistent alignment along the ideal 1:1 line, indicating that the surrogate models capture the underlying relationships between physicochemical parameters and methane performance with high fidelity. The uncertainty band around the predictions reveals broader intervals at extreme methane yield values, which reflects increased model uncertainty when extrapolating outside dense data regions. This behavior is expected in biological systems where extreme operational conditions or unusual feedstock characteristics introduce higher variability. In the mid-range (240–300 mL CH_4/g VS), the predictions fall within tight intervals, demonstrating strong confidence and stable response behavior. The combined visualization of mean prediction and confidence region confirms that the surrogate models not only predict methane yield accurately but also provide reliable uncertainty estimation essential for informed decision-making in virtual experimentation and digital prototyping.

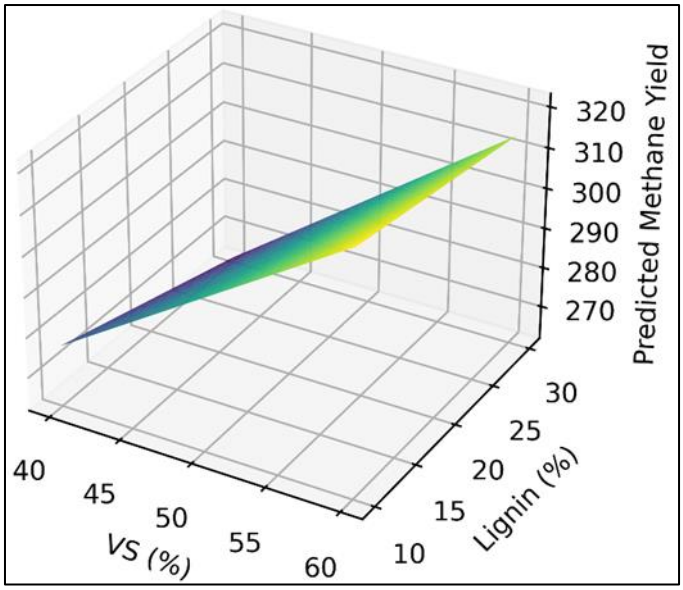

Figure 8 Surrogate model response surface (DNN)

The 3D response surface generated by the DNN surrogate, illustrating how methane yield varies with VS and lignin content is shown in figure 8. The surface demonstrates the model's capability to capture nonlinear digestion dynamics, including interactive effects where yield increases with higher VS content but decreases with increasing lignin concentration. The downward slope along the lignin axis clearly represents the inhibitory structural complexity of lignified biomass, while the upward gradient along VS indicates enhanced substrate availability. The smooth curvature of the surface also highlights the DNN's ability to produce realistic and biologically consistent response patterns without abrupt discontinuities. Such response surfaces are critical in surrogate simulation because they allow operators to visually inspect how changes in feedstock composition influence methane performance, enabling rapid scenario analysis, optimal feedstock blending strategies, and threshold identification for maximizing methane yield. This figure confirms the surrogate model's strength in replicating real AD behavior using computational simulation.

Overall, the results confirm that the proposed AI-driven surrogate framework provides an accurate, computationally efficient, and biologically consistent alternative to traditional experimental methane yield assessment. The combined strengths of DNN, GPR, RF, and SVR enable rapid simulation of AD performance under diverse conditions, supporting real-time decision-making, feedstock optimization, and digital prototyping of biogas systems. The surrogate models effectively capture nonlinear digestion dynamics, quantify prediction uncertainty, and deliver robust sensitivity interpretations, establishing a strong foundation for integrating surrogate-based intelligence into advanced AD process control and digital twin architectures. These findings demonstrate the significant potential of AI-enabled surrogate modeling to accelerate research, reduce experimental burdens, and enhance operational efficiency in biomass-to-energy conversion systems.

5. Conclusion

This study presented a novel AI-driven surrogate simulation framework designed to emulate anaerobic digestion behavior and rapidly predict methane performance without the need for repeated laboratory experimentation. By integrating DNN, GPR, RF–based surrogate modeling, and Support Vector Regression, the framework successfully captured the nonlinear, multi-dimensional interactions governing AD processes. The surrogate models demonstrated high predictive fidelity, with DNN and GPR providing superior approximation accuracy and uncertainty quantification, while RFS and SVR offered robust and computationally efficient alternatives. The developed surrogate workflow enables instantaneous simulation of methane yield responses under varying feedstock compositions and operating conditions, supporting virtual experimentation, parameter sensitivity analysis, and optimization-driven decision-making. The results show that AI-ML surrogate models can effectively replace a significant proportion of physical BMP trials, substantially reducing experimental time, cost, and resource requirements. Overall, this work establishes a scalable foundation for intelligent AD system design, real-time biogas plant optimization, and the development of advanced digital twins for biomass-to-energy systems. Future work will focus on expanding the surrogate framework to incorporate dynamic digestion kinetics, multi-objective optimization, and integration with automated control architectures for next-generation smart biogas facilities.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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