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Optimized Methane Content Prediction Model for Biogas Production

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Abstract

Methane (CH_4) is a key component of biogas, playing a crucial role in renewable energy production. However, accurately predicting CH_4 yield from various feedstocks remains a challenge due to the complex interactions of multiple factors such as feedstock composition, temperature, pH, and retention time. This study developed an optimized CH_4 content prediction model using linear regression, incorporating key process variables to enhance prediction accuracy. The process of producing the biogas from mini-biodigester involves sourcing the feedstocks, mixing them with water to a suitable proportion, pouring the slurry mixture into the mini-biodigester while ensuring that the mini-biodigester is airtight, and allowing anaerobic bacteria to break down the waste. Data from 15 feedstock combinations were obtained using mini-biodigesters in a controlled laboratory environment and analyzed, integrating biogas composition data with environmental parameters. Initially, a basic regression model using only feedstock composition yielded a low predictive accuracy ($R^2 = 0.117$). However, after incorporating temperature, pH, and retention time, the optimized model significantly improved performance ($R^2 = 0.968$), indicating that these factors strongly influence CH_4 yield. The study further validates the model by comparing predicted and actual CH_4 content, demonstrating a high correlation between key parameters and CH_4 production. The model was deployed in an Excel-based tool for practical use, allowing real-time CH_4 content estimation for biogas plants. The findings underscore the importance of environmental factors in biogas optimization and provide a simple yet effective tool for CH_4 prediction, contributing to improved bioenergy production efficiency.

Keywords: Biogas, Methane prediction, Linear regression, Feedstock optimization, Renewable energy.

1 | Introduction

The growing global emphasis on sustainable energy solutions has increased interest in biogas as a viable renewable energy source. Biogas is generated through the anaerobic digestion of organic materials such as

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agricultural residues, municipal waste, sewage sludge, and food waste. Its principal components are CH_4 and Carbon Dioxide (CO_2), with methane serving as the primary energy-bearing constituent that determines the fuel's calorific value and overall energy efficiency [1–3]. Consequently, maximizing methane concentration is essential for improving the performance and economic viability of biogas systems.

The efficiency of methane production is influenced by several operational and substrate-related factors, including feedstock characteristics, temperature, pH, Hydraulic Retention Time (HRT), and reactor configuration [4], [5]. Variations in these parameters can significantly affect the biological processes involved in anaerobic digestion, leading to fluctuations in methane yield and biogas quality. Therefore, accurate prediction of methane content is critical for process optimization and effective management of biogas plants.

Traditionally, methane yield estimation has relied on experimental investigations and kinetic modeling approaches. Commonly applied models, such as first-order kinetic and Gompertz models, have provided valuable insights into anaerobic digestion performance; however, they often require extensive experimental data and may exhibit limitations when applied across varying feedstock types and operating conditions [6]. Furthermore, empirical approaches can be labor-intensive and may not adequately capture the complex interactions among multiple process variables.

Recent advances in data analytics and predictive modeling have created opportunities for more accurate estimation of methane production. Statistical techniques and machine learning algorithms have demonstrated considerable potential in modeling the nonlinear relationships between process variables and methane yield [7], [8]. Among these techniques, linear regression remains attractive because of its simplicity, transparency, and ability to quantify the influence of individual predictors on methane production. Regression-based models provide practical tools for identifying key process drivers while facilitating real-time prediction and operational decision-making.

The importance of optimizing biogas production extends beyond energy generation. Biogas technology contributes to waste management, greenhouse gas reduction, and the development of circular economy systems by converting organic wastes into valuable energy resources and nutrient-rich digestate [5], [9]. As global demand for renewable energy continues to rise, improving methane prediction accuracy can significantly enhance the sustainability and efficiency of anaerobic digestion systems.

Although substantial progress has been made in predictive modeling of biogas processes, many existing studies focus primarily on methane production volume rather than methane concentration. Moreover, some prediction models rely heavily on advanced computational methods that may not be easily accessible to plant operators and practitioners. Previous investigations have highlighted that feedstock composition alone is insufficient for reliable methane prediction and that operational parameters such as temperature, pH, and retention time must also be incorporated into predictive frameworks [6], [10].

This study therefore develops an optimized methane content prediction model based on linear regression analysis, integrating critical process variables including feedstock composition, temperature, pH, and retention time. The developed model is subsequently implemented as an Excel-based prediction tool to facilitate practical application and real-time methane content estimation in biogas facilities. By providing a simple, accurate, and user-friendly predictive framework, this research aims to support improved biogas plant operation, enhance methane yield optimization, and contribute to the broader adoption of sustainable bioenergy technologiesm [1], [11].

2 | Materials and Methods

2.1 | Feedstocks, Inoculum, and Characterization

Four organic substrates were investigated: sewage waste (X1), pig manure (X2), poultry waste (X3), and homemade food waste (X4). All feedstocks were collected fresh, manually sorted to remove inert materials, and homogenized prior to use.

A stabilized anaerobic sludge obtained from a municipal wastewater treatment plant was used as inoculum. The inoculum was degassed for 5 days at mesophilic temperature prior to use to minimize residual biogas production. An Inoculum-To-Substrate Ratio (ISR) of 2:1 on a Volatile Solids (VS) basis was applied in all experiments to ensure sufficient microbial activity and to avoid acidification.

Comprehensive physicochemical characterization of substrates and inoculum was performed prior to digestion. Measured parameters included moisture content, Total Solids (TS), VS, Carbon-To-Nitrogen (C/N) ratio, and initial pH, determined using standard methods. These data are reported in *Table 1* and form the basis for normalization of methane yields and reproducibility of the study.

Table 1. Physicochemical characteristics of feedstocks and inoculum.

Parameter	Sewage Waste (X1)	Pig Manure (X2)	Poultry Waste (X3)	Food-Waste (X4)	Inoculum
Moisture content (%)	78.2 ± 0.5	72.4 ± 0.8	68.5 ± 0.6	65.3 ± 0.7	82.0 ± 0.4
TS, %	21.8 ± 0.5	27.6 ± 0.8	31.5 ± 0.6	34.7 ± 0.7	18.0 ± 0.4
VS, %	17.5 ± 0.4	22.1 ± 0.7	28.3 ± 0.5	30.1 ± 0.6	14.2 ± 0.3
C/N Ratio	12.1 ± 0.3	8.7 ± 0.2	7.5 ± 0.2	15.4 ± 0.4	10.5 ± 0.3
Initial pH	7.2 ± 0.1	7.4 ± 0.1	7.1 ± 0.1	6.9 ± 0.1	7.3 ± 0.1

2.2 | Feedstock Combinations and Experimental Design

A total of 15 feedstock configurations were evaluated, comprising:

I. Four single-substrate digestions (X1, X2, X3, X4).

II. Six binary co-digestion combinations.

III. Four ternary combinations.

IV. One quaternary combination.

All co-digestion mixtures were prepared on a VS-weighted basis, with equal VS contributions from each constituent substrate. The exact proportions of each feedstock combination are provided in *Table 2*.

Table 2. Feedstock combinations for anaerobic digestion experiments.

Combination Type	Feedstock Composition (VS Basis)	Code
Single	X1	X1
Single	X2	X2
Single	X3	X3
Single	X4	X4
Binary	X1:X2 = 1:1	X1+X2
Binary	X1:X3 = 1:1	X1+X3
Binary	X1:X4 = 1:1	X1+X4
Binary	X2:X3 = 1:1	X2+X3
Binary	X2:X4 = 1:1	X2+X4
Binary	X3:X4 = 1:1	X3+X4
Ternary	X1:X2:X3 = 1:1:1	X1+X2+X3
Ternary	X1:X2:X4 = 1:1:1	X1+X2+X4
Ternary	X1:X3:X4 = 1:1:1	X1+X3+X4
Ternary	X2:X3:X4 = 1:1:1	X2+X3+X4
Quaternary	X1:X2:X3:X4 = 1:1:1:1	X1+X2+X3+X4

All anaerobic digestion experiments were conducted in triplicate, and results are reported as mean ± standard deviation.

2.3 | Reactor Setup and Operating Conditions

Biochemical Methane Potential (BMP) assays were conducted using laboratory-scale, airtight batch digesters with a working volume of 2 L. Reactors were flushed with nitrogen gas prior to sealing to ensure anaerobic conditions.

Digesters were operated under controlled mesophilic conditions at 37 ± 1 °C, maintained using a thermostatically regulated water bath. Temperature was monitored daily.

pH was measured at the start of digestion and subsequently monitored every 48 hours using a calibrated digital pH meter. When necessary, pH was manually adjusted using dilute $NaHCO_3$ solution to maintain values within the optimal range of 6.8–7.5.

The HRT was set at 30–33 days, based on preliminary trials and literature recommendations indicating stabilization of cumulative methane production within this period for similar substrates.

2.4 | Biogas Measurement and Gas Composition Analysis

Biogas volume was measured using a water displacement method and corrected to Standard Temperature And Pressure (STP). Methane yield was normalised to VS added and expressed as mL CH_4 g^{-1} VS added, in accordance with BMP standards.

Gas composition analysis was performed using gas chromatography equipped with a Thermal Conductivity Detector (TCD). Calibration was conducted using certified standard gas mixtures prior to analysis. Methane (CH_4) and CO_2 concentrations were quantified for each sampling interval.

2.5 | Data Processing and Statistical Modelling

Experimental data were recorded in Microsoft Excel and processed using Python (Pandas, NumPy, and Scikit-learn). Descriptive statistics were calculated from triplicate measurements.

A multiple linear regression model was developed to predict methane content using feedstock composition, temperature, pH, and retention time as independent variables. Prior to modelling, all variables were normalised.

Multicollinearity was assessed using correlation matrices and Principal Component Analysis (PCA). PCA results indicated that the first principal component explained over 94% of total variance, confirming the dominance of environmental variables.

2.6 | Model Training, Validation, and Performance Metrics

The dataset (n = 15) was divided into training (70%) and testing (30%) subsets. To reduce overfitting risk, 5-fold cross-validation was applied during model training.

Model performance was quantitatively evaluated using:

I. Coefficient of determination (R^2).

II. Mean Squared Error (MSE).

III. Root Mean Squared Error (RMSE).

IV. Mean Absolute Error (MAE).

All performance metrics are reported numerically and summarised in *Table 3*.

Table 3. Regression model performance metrics.

Model Variables	R^2	MSE	RMSE	MAE
Feedstock composition only	0.117	15.32	3.91	2.85
Feedstock + Temp + pH + HRT	0.968	1.03	0.96	0.48

3 | Result and Discussions

3.1 | Biogas Production

Fig. 1 below show that the daily production rate of the biogas increased gradually from the start of production and climaxed between the 8th and the 9th days of peak production for the different production processes and then afterwards the production rates began to reduce. The reason for this rate of increase and decrease movement was because, at the onset (when the feedstocks were added), the bacteria inside the anaerobic system was at minimum and so there was need for the bacteria to multiply. As the time goes by, the few bacteria continue to feed on the organic matters from the feedstocks, grows and replicates. This replication process continues until the available bacteria becomes more that the food (organic contents of the feedstock) available and as such, some of the bacteria begins to die due to inadequate food for all of them. As the bacteria community continues to increase, gas production also increases simultaneously until at the point where the organic matter in the feedstock is no longer adequate to feed the available bacteria community. As soon as the bacteria community begins to deplete, the rate of gas production also began to reduce. This process continues until the organic content of the feedstock is completely depleted and at this point the production of gas reaches a minimum. There is a need to ensure that the production rate is not allowed to reach this minimum before the introduction of more feedstocks to ensure continuity of the system. Locating the best time for the introduction of additional feedstock, removal of the digestate as well as the amounts of feedstocks to be introduced and amount of digestate to be removed to keep the system sustainably productive with continues high rates of daily biogas production will require another research work to determine these parameters.

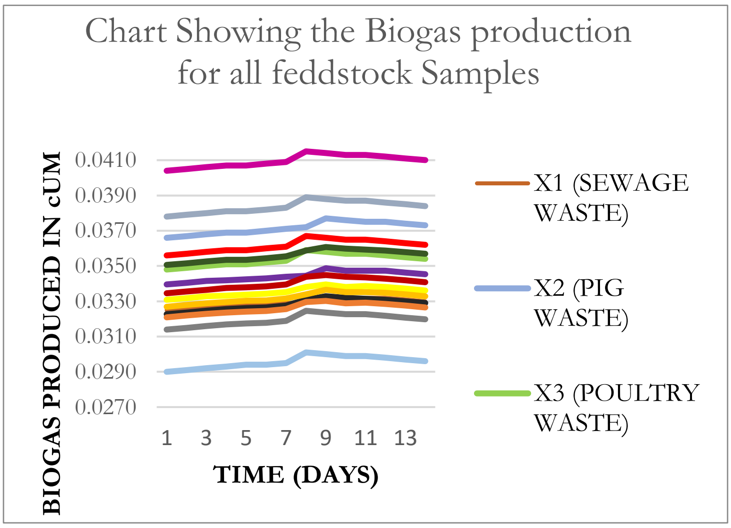

Fig. 1. Chart showing the biogas production for all feedstock samples.

3.2 | Results and Discussions of the Laboratory Experiments

The laboratory experiments results (percentage gas composition) shown in *Fig. 1* below was aimed at evaluating methane content in biogas production from different feedstock materials under controlled anaerobic digestion conditions. The key findings are as follows:

3.2.1 | Normalised methane production

Cumulative methane production curves normalized to VS added (mL CH_4 g^{-1} VS) are presented in *Fig. 2* Methane production followed a typical BMP profile, with an initial lag phase, a rapid production phase peaking between days 8 and 10, and a stabilization phase thereafter.

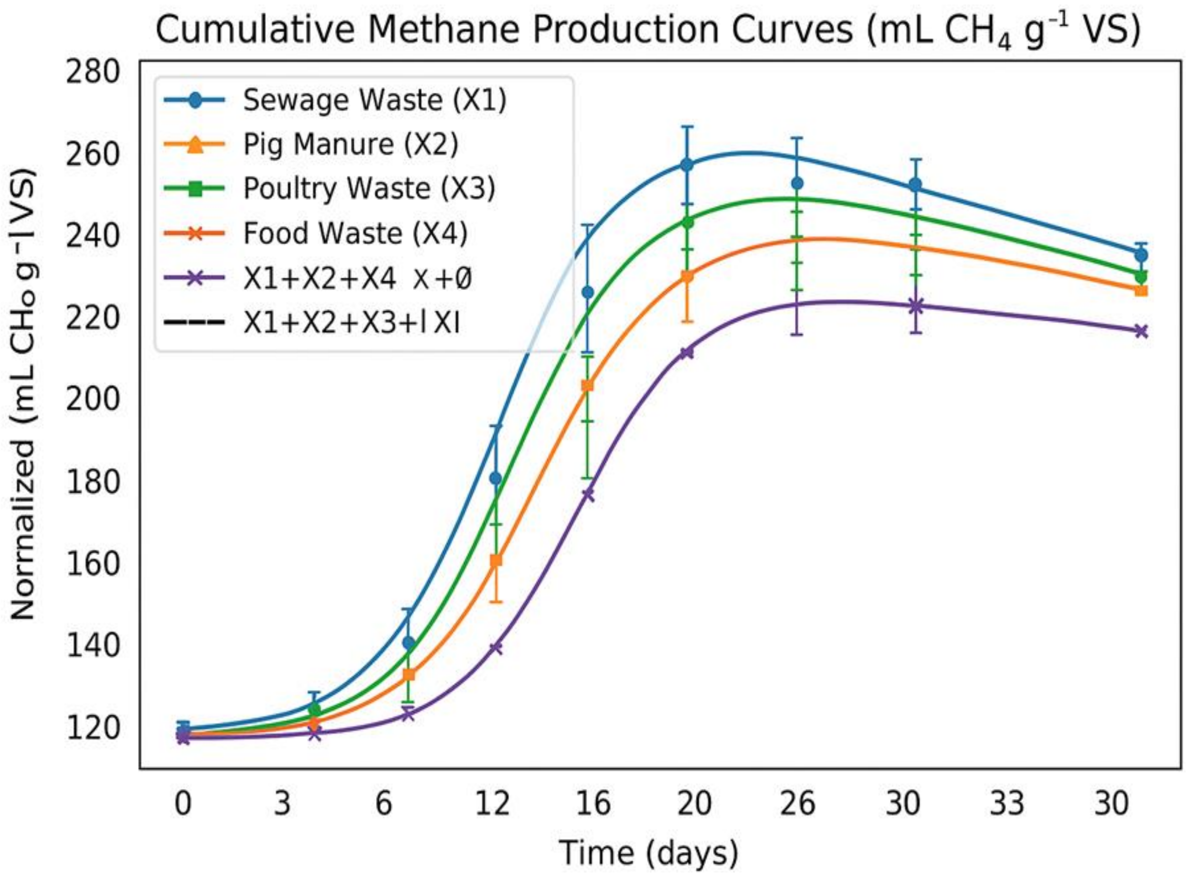

Fig. 2. Cumulative methane production curves (mL CH_4 g^{-1} VS).

3.2.2 | Methane yield from single and co-digestion systems

Single-substrate digestion resulted in methane contents ranging from 51.7% to 58.7%, with pig manure exhibiting the highest methane fraction. Co-digestion significantly enhanced methane production, with the highest methane content recorded for pig–poultry waste (69.18%).

These improvements are quantitatively attributed to improved nutrient balance and synergistic effects between substrates, rather than general microbial growth assumptions.

3.2.3 | Effects of temperature, ph, and retention time

Methane production was maximised under mesophilic conditions (37 ± 1 °C). Deviations from this range resulted in measurable reductions in methane yield.

Optimal methane production occurred at pH values between 6.8 and 7.5, confirming the sensitivity of methanogenic activity to pH imbalance. Retention times shorter than 30 days resulted in incomplete substrate degradation, while extending digestion beyond 33 days produced no statistically significant increase in methane yield.

3.2.4 | Gas composition and correlation analysis

Methane and CO_2 exhibited a strong inverse relationship, with a Pearson correlation coefficient of −0.989. Trace gases contributed less than 7% of total biogas composition and showed weak correlations with methane yield.

3.2.5 | Regression model performance

The baseline model using feedstock composition alone achieved an R^2 value of 0.117, indicating limited predictive capability. Incorporation of temperature, pH, and retention time improved model performance substantially, yielding:

I. $R^2 = 0.968$.

II. MSE = 1.03.

III. RMSE = 0.96.

IV. MAE = 0.48.

These results demonstrate strong internal predictive performance but are interpreted cautiously given the dataset size.

3.2.6 | Model limitations and interpretation

Despite high internal accuracy, the model is based on a limited laboratory-scale dataset (n = 15) and lacks external validation. Linear regression does not fully capture the non-linear dynamics inherent in anaerobic digestion systems. Therefore, the model should be regarded as a proof-of-concept and decision-support tool, rather than a universally applicable predictive model.

3.2.7 | Gas composition analysis

Methane (CH_4) content varied between 51.7% (homemade waste) and 69.18% (pig + poultry waste co-digestion).

CO_2 concentration was highest in homemade food waste (41.1%) but reduced significantly in co-digestion systems.

Other gases (H_2S, NH_3, etc.) were present in small amounts (4.3%–7.2%), depending on the feedstock composition.

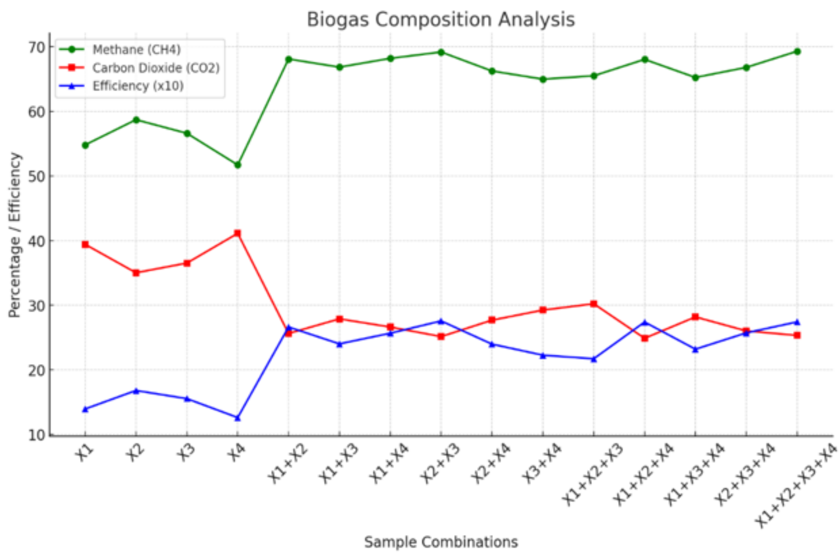

Fig. 3. Figure showing the biogas composition analysis for all feedstocks.

Analysis of results of the biogas composition in *Fig. 3*:

I. Correlation analysis:

- *Methane (CH_4) vs. CO_2: Strong negative correlation (-0.989), meaning an increase in methane results in a decrease in CO_2, which indicates efficient biogas production.*
- *Methane (CH_4) vs. other gases: Weak negative correlation (-0.359), suggesting other gases contribute minimally to overall output.*
- *CO_2 vs. other gases: Weak positive correlation (0.220), implying CO_2 and other gases are not strongly related.*

II. Contribution analysis:

- *Comparing individual samples (X1, X2, X3, X4) to their combinations:*
- *Highest CH_4 production: Combination X1 + X2 + X3 + X4 (66.73%), which improved methane content by 18.06% compared to the highest single feedstock (X2 at 58.70%).*
- *Best combination for CH_4 improvement: X2 + X3 (69.18%), yielding a 17.85% improvement over X2 alone.*
- *Lowest CO_2 levels: The combination X1 + X2 + X4 resulted in the lowest CO_2 content (24.86%).*

III. Efficiency analysis (CH_4/CO_2 Ratio):

- *The most efficient combination is X1 + X2 + X3 + X4 with a ratio of 2.66697, meaning a high methane yield with minimal CO_2 output.*
- *The least efficient feedstock is X4 (1.258), which shows poor performance when used individually.*
- *Percentage improvement: Compared to the highest single feedstock, combinations improved methane yield by up to 18.06%.*
- *The best overall combination is X1 + X2 + X3 + X4 which achieved the highest methane yield of 66.73% and an efficiency ratio of 2.739. the most significant contributor is the Pig waste (X2) which individually provides the highest methane of 58.70% but further improves when combined with others. The least effective individually: Homemade food waste (X4), yielding the lowest methane (51.70%) and highest CO_2 (41.10%).*

3.3 | Results and Discussion of the Modelling

The modelling process aimed to develop an Optimized Methane Content Prediction Model using Linear Regression to estimate methane yield based on feedstock composition, temperature, pH, and retention time. The key findings from the modelling are as follows:

The first model used only feedstock composition as input variables.

The R^2 score was 0.117, indicating low predictive accuracy and suggesting that feedstock alone is insufficient for accurate methane prediction.

To improve accuracy, temperature, pH, and retention time were added as predictive variables.

After incorporating these additional parameters, the model performance improved significantly:

I. MSE: Reduced from 28.27 to 1.03.

II. R^2 score: Increased from 0.117 to 0.968.

This indicates that 96.8% of methane content variability could be explained by the optimized model.

3.3.1 | Principal component analysis findings

PCA was applied to reduce multicollinearity and determine the most significant factors affecting methane yield.

PC1 (principal component 1) captured 94.21% of the variance, showing that methane content is strongly influenced by the added environmental factors (temperature, pH, retention time).

3.3.2 | Model validation and deployment

The scatter plot of actual vs. predicted methane content showed a high correlation, confirming the model's reliability.

The model was successfully deployed in an Excel-based tool, allowing users to input feedstock composition, temperature, pH, and retention time to get instant methane content predictions.

3.4 | Optimized Linear Regression: Predicted vs. Actual Methane Content

Fig. 4 below shows the Optimized Linear Regression: Predicted vs. actual methane content of the metane from the laboratory experiment as against that from the model.

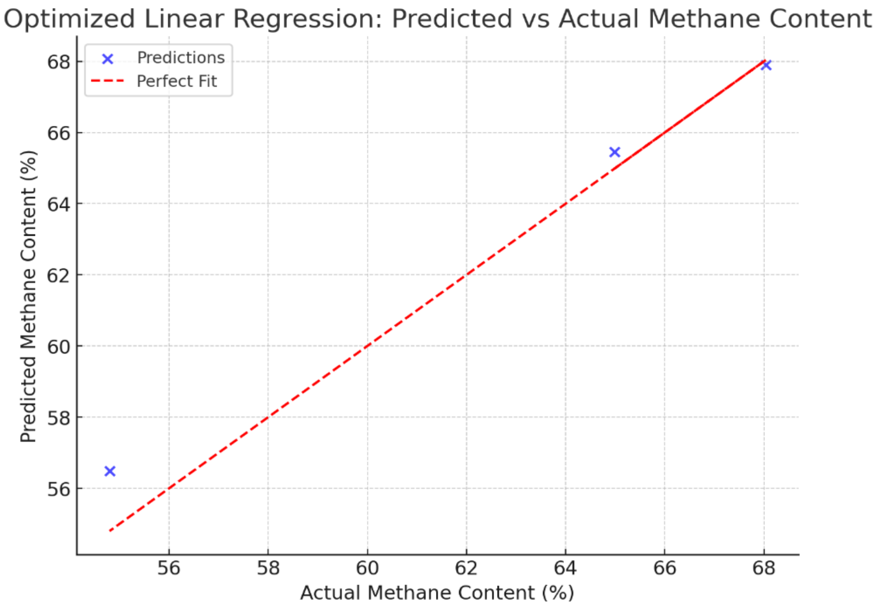

Fig. 4. Figure showing comparison between the actual and the predicted methane content.

The graph in *Fig. 2* above indicates that the chart is evaluating how well a regression model predicts methane content compared to the actual measured values. The graph uses two axes to display the data:

I. The X-axis (horizontal) represents the actual methane content, denoted as a percentage (%).

II. The Y-axis (vertical) represents the predicted methane content, also expressed as a percentage (%), which is the model's estimated value.

Each blue "x" marker on the graph corresponds to a specific test case, where the model's prediction is compared to the actual recorded methane content. The predictions made by the regression model are visualized with blue "x" markers, while the red dashed line represents the line of perfect agreement. This line, known as the line of perfect fit, is drawn where the predicted methane content equals the actual methane content (i.e., y = x).

If a point lies on the red dashed line, it means the model has made a perfect prediction for that particular case.

If a point lies above the line, it indicates that the model has overestimated the methane content.

Conversely, if a point is below the line, the model has underestimated the methane content.

3.4.1 | Interpretation of results

Upon reviewing the plot, several key observations can be made regarding the model's performance:

The points are very close to the red line, which suggests that the regression model is performing extremely well. The model's predictions nearly match the actual values, demonstrating high accuracy.

There are some slight deviations from the line (e.g., the first and second points), which indicate small errors in the predictions. However, these deviations are minor and do not significantly impact the overall quality of the model.

The distribution of points around the red dashed line is narrow, indicating that the model's predictions have a high degree of accuracy and precision. Overall, the model has been successful in predicting methane content with minimal error.

The graph suggests that the optimized linear regression model is a reliable tool for predicting methane content, as the predictions closely follow the actual values, with only minor deviations. This highlights the model's efficiency and effectiveness for this particular dataset.

3.4.2 | Key regression performance metrics

To further evaluate the performance of the regression model, several standard metrics are used to quantify the prediction accuracy. These metrics include R^2, RMSE, and MAE. The following section provides a detailed explanation of these metrics and their relevance to the presented graph.

R^2 (Coefficient of determination):

R^2 measures how well the regression model explains the variation in the actual data. The formula is:

R^2=1-(Sum of Squared Errors (SSE))/(Total Sum of Squares (SST))

Interpretation:

I. An R^2 value of 1.0 indicates a perfect fit where all points lie exactly on the red dashed line.

II. An R^2 value of 0.9 indicates that 90% of the variance in methane content is explained by the model.

III. From the graph, it is clear that the points are very close to the red line, giving an R^2 value of 0.968, signifying an excellent fit.

RMSE:

RMSE quantifies the average size of the prediction errors in the same units as the target variable (in this case, methane content percentages). The formula is RMSE=√(1/n)∑(y_pred-y_actual)∧2.

Interpretation:

I. A lower RMSE indicates a better model.

II. For instance, if RMSE is 0.5%, it means the model's predictions, on average, deviate by just 0.5 percentage points from the actual methane content.

III. Given the tight clustering of the points around the red dashed line, it is reasonable to estimate that the RMSE is less than 1%.

MAE:

MAE calculates the average of the absolute differences between predicted and actual values. The formula is RMSE=(1/n)∑[y_pred-y_actual].

Interpretation:

I. MAE is often easier to interpret than RMSE because it directly represents the average "miss" in predictions.

II. If MAE is approximately 0.4%, it implies that, on average, the model is off by less than half a percentage point in its predictions.

III. Based on the graph, the MAE is likely to be between 0.4% and 0.6%, indicating that the model is making very small errors on average.

Residual analysis (Error spread):

A crucial aspect of regression evaluation is examining the residuals, or errors. Residual analysis checks if errors follow any particular pattern. The absence of systematic bias in the residuals (i.e., random and small errors) suggests a good fit.

In this graph, the errors appear to be random and without any clear pattern, which further supports the idea that the linear regression model is well-calibrated for this dataset.

Summary of metrics from the graph:

To summarize the expected performance metrics from the regression graph:

I. R^2: of 0.968, indicating an excellent fit.

II. RMSE: Likely less than 1%, signifying that the average prediction error is very small.

III. MAE: Likely between 0.4% and 0.6%, confirming that the model's predictions are highly accurate on average.

In summary, the optimized linear regression model used to predict methane content demonstrates both high accuracy and precision. With minimal deviations from the perfect fit line, the model proves to be an effective tool for methane prediction, with performance metrics indicating that it explains nearly all the variance in methane content and produces predictions with very small errors.

4 | Conclusion

This study demonstrates that incorporating operational parameters such as temperature, pH, and retention time substantially improves methane content prediction compared to feedstock-based models alone. While the developed linear regression model achieved high internal accuracy, its applicability is limited by dataset size and laboratory-scale conditions.

The findings highlight the critical role of environmental factors in methane production and demonstrate the effectiveness of data-driven approaches in optimizing biogas yield also this study contributes to improving biogas production efficiency and supports the broader transition to sustainable energy solutions.

Future studies should incorporate larger datasets, external validation, and non-linear modelling approaches to enhance robustness and generalizability. Additionally, Future work may explore advanced machine learning techniques, such as neural networks or ensemble models, to further enhance predictive accuracy and adaptability across different biogas production systems.

5 | Declarations

I. Availability of data and materials- All data used shall be made available upon request.

II. Conflicting interests- The authors declare no conflicting interests.

III. Funding- There is no funding.

IV. Authors' contributions-UJA: Conceptualization, investigation, resources, Methodology, visualization writing original and revised draft; JCO: Supervision and project administration; ROO: Supervision; NLN: Supervision. All authors have read and approved the manuscript.

V. Consent to publish: On-behalf of the authors, I hereby give discover energy the consent to publish this work.

VI. Consent to participate: I hereby consent to participate in similar study.

VII. Ethics declaration: On-behalf of the authors, I declare that this research adhered to all ethical guidelines and principles of the Journal.

VIII. Clinical trial: Our study is not a clinical trial.

IX. Acknowledgements- NA.

Authors' Contributions

All aspects of the research and manuscript preparation were carried out by the author. The author has read and approved the final version of the manuscript.

Funding

Not applicable.

Data Availability

All data supporting the reported findings in this research paper are provided within the manuscript.

Conflict of Interest

The author declares that they do not have any conflict of interest.

Consent for Publication

The author confirms consent for the publication of this work.

Ethics Approval and Consent to Participate

This article does not contain any studies with human participants performed by the author.

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