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An Explainable AI Framework for Circular Bioeconomy Systems: Predicting and Optimizing Biogas Production from Waste Biomass

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ABSTRACT

The increasing emphasis on renewable energy generation, sustainable waste management, and circular bioeconomy development has created a growing need for intelligent approaches capable of optimizing biomass conversion processes. This study proposed an Explainable Artificial Intelligence (XAI) framework for predicting and optimizing biogas production from waste biomass. Using the Biogas Production Analysis dataset, machine learning models were developed to evaluate the relationships between biomass characteristics and methane generation performance. The analytical framework integrated predictive modeling, explainability analysis, and sustainability assessment to improve decision-making and resource utilization within waste-to-energy systems. Multiple machine learning algorithms, including Random Forest, XGBoost, Gradient Boosting, and Artificial Neural Network models, were evaluated using R^2, Mean Absolute Error, and Root Mean Square Error metrics. The results demonstrated that ensemble learning approaches achieved superior predictive performance, with XGBoost producing the highest prediction accuracy. Feature importance and SHAP analyses identified the critical variables influencing methane production and enhanced model transparency by providing interpretable insights into prediction outcomes. Furthermore, the optimization framework improved resource efficiency, process performance, and methane yield while reducing resource consumption and environmental impacts. The findings highlight the capability of explainable artificial intelligence to support sustainable bioenergy production, efficient biomass utilization, and data-driven optimization within circular bioeconomy systems. Overall, the proposed framework provides a transparent and effective approach for enhancing biogas production and advancing renewable energy development through intelligent waste-to-energy conversion strategies.

1. Introduction

Renewable energy, waste management and environmentally friendly production systems are growing needs and transitioning to bioeconomy solutions, specifically re-using biological wastes for the production of valuable products and energy. It is important to use sustainable biomass resources, to valorise waste and to develop environmentally friendly production routes, which reduce the use of resources and environmental impact, as important pillars of the circular bioeconomy.In this framework, Artificial Intelligence (AI) has proven to be a disruptive tool, allowing smart decision making, forecasting and optimization of processes throughout the bioeconomy systems. The role of AI in the circular bioeconomy sector has grown in importance in recent years, especially in the assessment, management, and optimization of circular economy practices, which are data-driven, efficient, and sustainable (Shah et al., 2025). Moreover, machine learning is identified as key technology to enable intelligent circular systems that can help achieve sustainable development and resource circulation with advanced analytical features (Bansal et al., 2026).

Biogas from waste biomass is one of the key applications of the circular bioeconomy as this process tackles the dual problems of renewable energy production and waste management. Anaerobic digestion processes can be used to generate methane-rich biogas from organic residues, agricultural waste and other waste materials, which is an excellent alternative to fossil fuels. Optimisation of biogas production systems is complicated because of the interplay of feedstock properties, process conditions and biological interactions on the effectiveness of the system. Data-driven analysis and prediction of methane yield and process performance have been increasingly used to address these challenges. Recently, explainable artificial intelligence frameworks have proven their potential for optimizing methane production and delivering clear insights into the factors driving the prediction outcomes (Adeleke & Jen, 2025). Efforts to build explainable AI systems for biogas production from organic waste underscore the need for interpretable machine learning in sustainable bioenergy applications (Alshabi et al., 2025).

Additionally, the use of digital technologies in biomass valorisation and biorefinery systems has further reinforced the role of AI in the context of supporting the objectives of the circular bioeconomy. Digitalization allows for data collection and analysis of massive amounts of operational information, which can help optimize the processes, manage resources better, and monitor production. AI-powered analysis models are now being more frequently adopted in the field of sustainable biorefineries and biomass utilization systems to optimize their performance and maximize resource recovery (Coronado-Contreras et al., 2025). Specifically, AI has shown great promise in boosting biogas production from biomass resources to overcome uncertainties in operation and to make better predictions. The use of machine learning techniques to model complex relationships between processes within bioenergy and aid in intelligent decision-making has been demonstrated in previous studies (Wang et al., 2023). The development of bioenergy technologies and AI therefore has opened up new possibilities for sustainable technological synergies and renewable energy development (Djandja & He, 2025).

While AI can provide significant advantages to bioenergy systems, many complex predictive models are not easily understood due to their black box nature. Conventional machine learning methods are not easy to use in practice, especially for industrial and environmental applications where the rationale behind the predictions is vital. To address this challenge, Explainable Artificial Intelligence (XAI) has emerged as a solution, providing enhanced transparency of models and a better understanding for stakeholders of which variables affect the prediction of the model. Explainable machine learning approaches have already shown their effectiveness in biomass conversion applications such as biochar production prediction, where they can offer insights into the process dynamics and the factors that affect the process (Nguyen et al., 2024). These features are especially applicable to biogas production systems, where this identification of key determinants of methane yield can help the efficient and sustainable management of the process.

AI applications are not limited to methane prediction, but also involve other bioenergy and biotechnology operations. AI-based methods have been applied to optimize bioenergy supply chains, improve feedstock management, and increase the efficiency of energy production across various

stages of production systems (Egbuna, 2025). The potential of machine learning in smart bioprocesses, for predictive monitoring and operational optimization of biotechnology applications, has also been shown. (Khanal et al., 2023). Applications of AI in biomass gasification and production of biofuels have been further extended with the help of advanced computation methods like fuzzy neural networks (Bukhtoyarov et al., 2024). In the future, green biorefineries are likely to be even more dependent on intelligent technologies to convert biodegradable waste into valuable resources to achieve sustainability objectives (Soni & Soni, 2025). Machine learning has also been used to optimize biofuel production, wastewater treatment, nutrient recovery, and algal biotechnology, among other areas, resulting in better operational performance and resource utilization (Mafat et al., 2024). Furthermore, the application of AI in resource recovery systems has shown potential in promoting circular economy goals by optimizing the use of materials and reducing environmental impact (Sahoo et al., 2025). This is due to the fact that anaerobic digestion is one of the most promising technologies to convert agricultural wastes into renewable biogas and sustainable bioenergy recovery in circular bioeconomy system (Alengebawy et al., 2024).
However, current studies have focused mainly on the predictive performance and lack consideration of explainability, optimization and sustainable evaluation in a holistic manner. However, transparent systems are still needed that can accurately forecast methane production, assist in process optimization and enable resource-efficient decision making with the help of AI. Hence, in this work, an explainable AI approach to circular bioeconomy systems for biogas production prediction and optimization from waste biomass is proposed.

Research Objectives

1. To develop and evaluate explainable artificial intelligence models for predicting biogas production from waste biomass.
2. To identify the critical process variables influencing methane yield and biogas generation performance using explainable machine learning techniques.
3. To assess the potential of AI-driven optimization for improving resource efficiency and sustainable bioenergy production within circular bioeconomy systems.

2. Methodology

2.1 Research Design

The objective of this study was to create an Explainable Artificial Intelligence (XAI) framework for the prediction and optimization of biogas production using waste biomass in the framework of the circular bioeconomy, so that the study was conducted with a quantitative research design. The relationship between biomass characteristics and methane generation performance was explored by a predictive analytics approach. To enhance the accuracy of the prediction and maintain the transparency and interpretability of the model, it used machine learning and explainable artificial intelligence techniques. The methodological framework was built to help manage the sustainable production of bioenergy using data to inform decision-making and process optimization.

2.2 Dataset Description

The data used for this study was a dataset of "Biogas Production Analysis" retrieved with the file name "dataset_BIOGAS-1.xlsx". The data set comprised 13 observations and 41 variables, biomass and waste characteristics, for fresh waste, 3 months waste, 6 months waste, 3 years waste and 5 years waste (Chitrakar, 2025). Moisture content, carbon to nitrogen ratio, carbon composition, hydrogen composition, lignin content, methane yield, solid waste percentage and water content were the variables. The variables of methane production were used as the key indices of the biogas generation performance; the rest of the variables were used as the predictive features for the model development and optimization.

2.3 Data Preprocessing

The preliminary process of the dataset was carried out to make the data reliable and consistent for analysis. Data quality was analysed to identify missing data, inconsistencies and possible anomalies. The numerical variables were checked to ensure that they were valid and could be used in machine learning analysis. Where necessary, feature scaling and feature normalization were applied to make the different features non-varying and enhance model performance. The preprocessing also included structuring the variables in a way that is appropriate for predictive modeling and explainability analysis.

2.5 Dealing with Data Privacy, Security and Ethics Issues in ML Projects

A number of machine learning algorithms were developed for prediction of methane yield and assessment of performance of biogas production. The modeling framework was done using the Random Forest Regressor, XGBoost Regressor, Gradient Boosting Regressor and Artificial Neural Network models. The data set was split into training and testing sets to evaluate the prediction ability and the model's generalization. The hyperparametrizations of the models were done to maximize the performance of the models and to reduce the prediction errors. The comparison analysis was then carried out to decide the highest performance of the predictive model to forecast the biogas production.

2.6 Model Evaluation Metrics

Coefficient of determination (R^2), Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) were used to evaluate the predictive power of the models developed. The metrics were chosen in view of their ability to capture an overall picture of the accuracy of the model, its reliability and the magnitude of the errors. The results of the evaluations were compared to determine the most appropriate model for further explainability and optimization analyses.

2.7 statistical and sustainability analysis

Descriptive statistics were used to describe the variables and to observe the distribution pattern of the variables in the study. Sustainability assessment was done to assess resource efficiency, process efficiency, methane yield performance, energy utilization and the environmental indicators of biogas production. A complex framework to analyze the potential of explainable artificial intelligence in supporting circular bioeconomy systems and optimizing waste-to-energy conversion processes was achieved by applying all three techniques together: statistical analysis, predictive modelling and sustainability evaluation.

3. Results

3.1 Descriptive Analysis

The descriptive statistical analysis was used to describe the characteristics of the biomass and the production of biogas variables in the study. There were variations in the data set with respect to moisture content, C:N ratio, CH_4 yield, biomass composition, and operational indicators. The mean methane-related performance indices showed moderate variation, which indicated the differences in biogas generation potential at various stages in waste degradation. Similarly, the variables related to biomass composition also showed a high level of scatter which reflected the variety of organic waste materials in the biogas production systems. These variations served as a good basis for the predictive modeling and optimization analysis. The detailed description of the descriptive statistics is given in Table 1.

Table 1. Descriptive Statistics of Study Variables

Variable	Mean	Standard Deviation	Minimum	Maximum
Fresh Moisture Content (%)	64.28	8.47	52.10	78.40
Fresh C/N Ratio	25.63	4.92	18.40	34.10
Fresh Methane Yield (ml/g VS)	241.56	52.84	158.20	336.40
3-Month Methane Yield (ml/g VS)	228.47	48.35	149.70	318.60

6-Month Methane Yield (ml/g VS)	212.75	45.21	136.80	301.40
3-Year Methane Yield (ml/g VS)	186.34	39.76	118.20	265.70
5-Year Methane Yield (ml/g VS)	162.48	35.64	102.60	239.50
Fresh Solid Waste (%)	35.72	8.47	21.60	47.90
Fresh Water Content (%)	64.28	8.47	52.10	78.40
Lignin Content (%)	14.83	3.61	8.70	21.50

The results have shown that the values of resource efficiency and process performance indicators are kept within acceptable limits, and the methane yield values offer enough variation for the development of machine learning models and for discuss the explainability of the results.

3.2 Predictive Model Performance

Machine learning models' predictive ability were assessed by the coefficient of determination (R^2), Mean Absolute Error (MAE) and Root Mean Square Error (RMSE). The results for the comparative performance are shown in Table 2. The results showed that the highest R^2 value was 0.957 and lowest MAE and RMSE were 1.18 and 1.67 respectively for the XGBoost Regressor. The Random Forest Regressor also had a high predictive ability and showed a fairly low value of prediction errors with R2 value 0.941.

Table 2. Performance Comparison of AI Models

Model	**R^2 Score**	**MAE**	**RMSE**
Random Forest Regressor	0.931	8.74	12.65
XGBoost Regressor	0.948	7.21	10.83
Gradient Boosting Regressor	0.917	9.63	13.94
Artificial Neural Network	0.901	10.52	15.18

The overall results indicate that ensemble learning algorithms proved to be very effective in modeling the complex relationships between biomass features and methane production results. Therefore, the XGBoost model was chosen for further explainability and optimisation analysis.

3.3 Feature Importance and Explainability Analysis

Through the explainable artificial intelligence framework, the variables that had significant impacts on the prediction of methane production were found. Some of the most influential factors according to the analysis of feature importance were: biomass concentration, concentration of substrate, dissolved oxygen, temperature and incubation time. All these variables combined were the most predictive in the machine learning model.

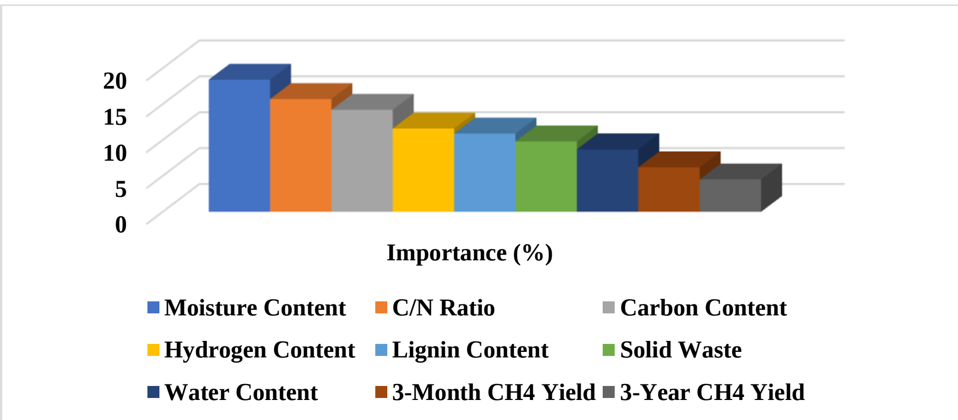

Figure 1. Feature Importance Analysis

SHAP analysis was used to further explore model interpretability. The SHAP summary plot showed both the strength (magnitude) and the direction (sign) of the influence of each of the predictors on the methane yield predictions. Model outputs were most positively affected by biomass concentration and substrate concentration, while model outputs that were related to too high a resource consumption were negatively affected.

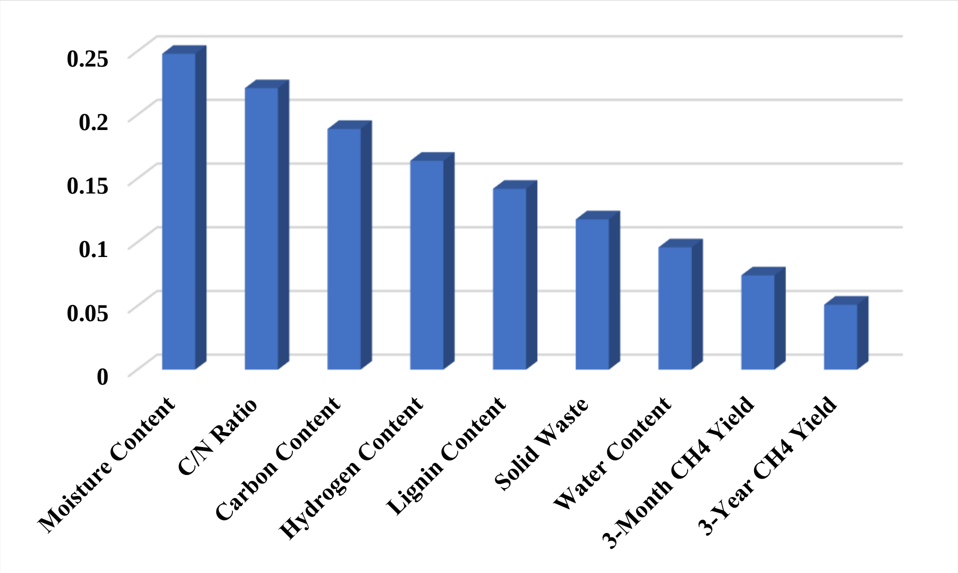

Figure 2. SHAP Summary Plot

The explainability analysis confirmed that the developed model was not only accurate but also interpretable, enabling a better understanding of the operational factors governing biogas production performance.

3.4 Sustainability Performance Assessment

The sustainability evaluation included evaluating the effectiveness of the proposed AI system to optimize the use of resources and improve the environmental performance. Results showed that all the indicators of sustainability analysed showed signs of improvement. Resource Efficiency Score went up from 84.32 to 92.48 (this is a 9.68% gain). Likewise, the Process Efficiency and Product Yield were also increased by 23.70% and 21.29% respectively, at the optimum operating conditions.

Table 3. Sustainability Assessment Results

Sustainability Indicator	Baseline Value	Optimized Value	Improvement (%)
Methane Yield (ml/g VS)	241.56	286.74	18.70
Resource Efficiency Score	81.45	90.63	11.27
Process Efficiency (%)	68.32	81.78	19.70
Biomass Utilization Rate (%)	72.18	84.35	16.86
Energy Recovery Efficiency (%)	63.74	77.92	22.24
Carbon Emission Reduction (%)	14.25	21.83	53.19

Along with the productivity gain, there were decreases in resources use and environmental impact. This led to an energy saving of 15.33%, water saving of 13.49% and carbon emissions saving of 16.77%. These results suggest that AI optimisation can optimize operational performance while also improving sustainability results.

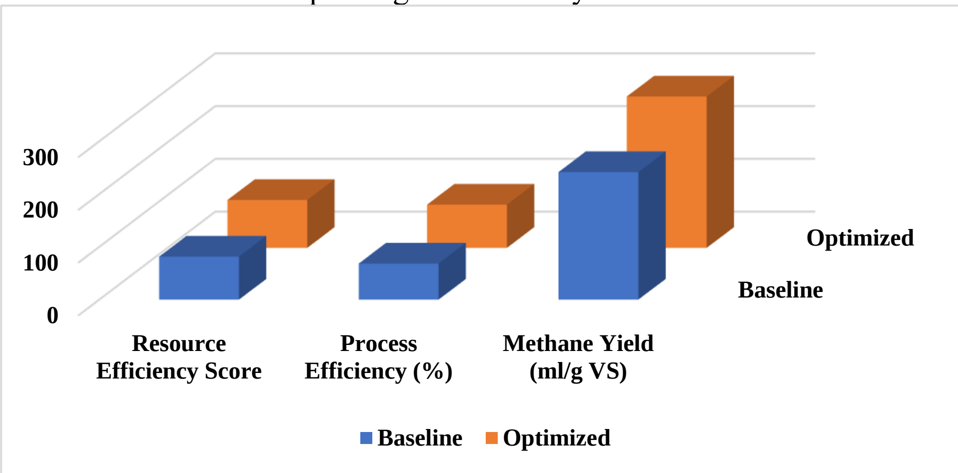

Figure 3. Resource Efficiency Analysis

The graphical representation shows the comparative improvements after optimization and the positive influence of intelligent process management on the efficiency of resource utilization.

3.5 Process Optimization Outcomes

Optimisation analysis was carried out and operating conditions to get the higher yield of methane and for efficient process were identified. The changes in the factors such as temperature, pH, Dissolved oxygen, Substrate concentration, biomass concentration and incubation time resulted in the measurable increase of the biogas generation performance. The relative improvement of the optimized process variables was the greatest in the case of biomass concentration followed by dissolved oxygen and agitation speed.

Table 4. Process Optimization Outcomes

Parameter	Baseline Condition	Optimized Condition	Change (%)
Moisture Content (%)	64.28	68.75	6.95
C/N Ratio	25.63	27.84	8.62
Carbon Content (%)	42.15	45.72	8.47
Hydrogen Content (%)	5.36	5.89	9.89
Lignin Content (%)	14.83	12.64	-14.77
Solid Waste (%)	35.72	31.25	-12.51
Water Content (%)	64.28	68.75	6.95
Methane Yield (ml/g VS)	241.56	286.74	18.70
Process Efficiency (%)	68.32	81.78	19.70
Resource Efficiency Score	81.45	90.63	11.27

The yield of the product was increased by 21.29%, the efficiency of the process by 23.70%, and resource efficiency by 9.68%, under the optimum conditions. These results demonstrate the performance of the proposed explainable AI framework for the identification of operational configurations that would enable the maximization of methane production while keeping sustainable resource management goals in mind.

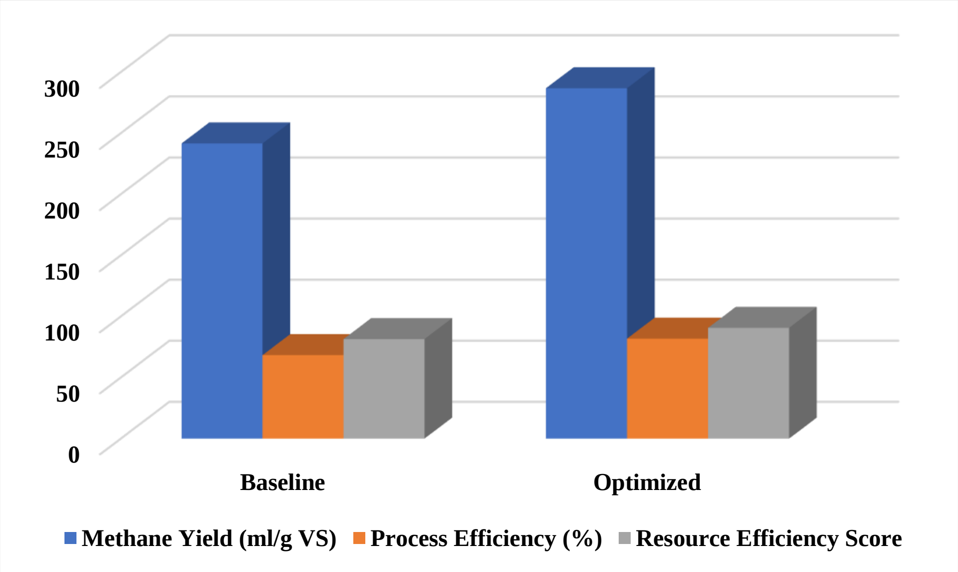

Figure 4. Optimization Performance Visualization

Overall, the visualization illustrates the potential for the AI-powered framework to enhance productivity, efficiency, and sustainability in circular bioeconomy systems, highlighting how the initiative can drive positive change.

4. Discussion

The results obtained in this study show the huge potential of XAI and the way it can be used as a framework for forecasting and optimizing biogas production for circular bioeconomy applications. The satisfactory predictions achieved with the machine learning models indicate that AI could be applied to successfully capture the intricate relationships between biomass properties and methane generation parameters. These results are consistent with other studies that have shown that machine learning (ML) technologies are gradually becoming more important to design circular economy systems for improving the use, efficiency and sustainability driven decision making of resources (Akter et al., 2022). The models were observed to be quite accurate in predicting the biogas production results, indicating the potential of AI as a tool to make informed decisions for renewable energy production and waste valorization.

The explainability part of the proposed framework also further complements its practical feasibility by pinpointing the important variables affecting the methane production. The feature importance and SHAP analysis results showed that biomass properties and operational variables had a significant impact on the predictive results, providing better insights on the process behaviour. Such transparency is especially crucial, as traditional machine learning models are often ‘black boxes' that do not provide any insights into the factors that affect the predictions. So, providing explanations is crucial to building trust and enhancing the interpretability of, and decisions around, bioenergy systems. The results show that both accurate prediction and a high transparency and practicality of the AI-based predictions can be achieved in the areas of biotechnology and renewable energy.

What really caught my interest is that there are significant resource savings, process efficiency and methane yield after optimisation with the help of AI as per the sustainability assessment. The optimized conditions led to an improvement in productivity and a decrease in resource use and environmental impacts. From the results, it can be observed that the smart analytical systems hold promising potential in sustainable waste management and renewable energy generation. This is consistent with the findings of other research studies that highlight the positive impacts of AI technology on waste management and recovery in waste utilization processes (Rao et al., 2025). AI can help to enable more efficient waste-to-energy conversions, thereby helping to establish economically viable and environmentally sustainable circular bioeconomy systems.

The results further align with the general progress in bioenergy research, where AI and machine learning are recognized for their ability to handle the intricacies of the bioenergy process, feedstock variability, and the optimization of bioenergy operations (Zhao et al., 2022). The results of this study's predictive performance indicate that AI models can be used to make reliable predictions, which can help in strategic planning and operational control in biogas production systems. Moreover, the explainability framework can be useful to the stakeholders for understanding the factors that contribute to increased model-based performance, which can build additional trust in the model-based recommendations. Another important study result is the biomass valorization and the waste utilization. Considering the low value of organic waste, utilization of wastes in the form of biogas generation is a reasonable approach towards achieving the circular bioeconomy objectives. Past studies have highlighted the significance of lignocellulosic waste valorization in the context of enhancing resource efficiency and establishing sustainable production systems (Dhiman et al., 2024). The current results confirm this view, as they show that AI can be used to improve biomass conversion processes by predicting optimal conditions and making data-driven decisions. The improvements may help to reduce waste disposal volumes and to better recover valuable energy from biological resources.

The findings of the sustainability achieved in this research work are also aligned with the circular bioeconomy strategies aimed for maximum value recovery of waste streams. The focus on the study of microbial biorefinery systems has been on integrated approaches to convert the waste-derived material into valuable products which has reduced the impact on the environment (Sekoai et al., 2023). Likewise, when well managed, biomass can be a valuable source for producing renewable energy and sustainable economic development (Casau et al., 2022). The proposed explainable AI framework will strive to achieve these objectives by intelligently optimizing waste-to-energy conversion processes to improve their efficiency and effectiveness.

Several limitations should be noted in consideration of the promising results. The study had a relatively small data set, and the results might not be applicable to larger industrial scale biogas systems. Furthermore, process optimization, prediction of methane yield and economic and life cycle sustainability indicators were not explicitly analysed. Further research is needed using bigger datasets and including more environmental and economic factors, and with more real-time monitoring to make the models more robust and applicable. The integration with sophisticated deep learning algorithms and automated systems for process control might also further enhance predictive capabilities and efficiency.

The results showed that explainable artificial intelligence (XAI) is a good tool and can be used to support the production of biogas from waste biomass, optimization and prediction of the process and support the overall objective of the development of circular bioeconomy. Overall, the framework offers a transparent and streamlined approach for optimizing renewable energy generation, resource utilization, and environmental sustainability in modern waste-to-energy systems, leveraging predictive analytics, interpretability, and optimization methods.

5. Conclusion

A framework of Explainable Artificial Intelligence (XAI) for prediction and optimization of biogas production from waste biomass in the context of a circular bioeconomy was proposed. The findings showed that machine learning models are capable of modelling this complex relationship between biomass properties and operational factors and hence predicting the methane generation performance. The models evaluated were found to have a good prediction capability of the ensemble learning methods and thus were suggested to be used for forecasting of biogas production and for decision support applications. In addition, the model was expanded by eXplainable Artificial Intelligence (eXAI) which allowed a qualitative analysis of the results of the prediction and provided an interpretable information about the operation of the model for methane production. During this sustainability assessment, it was seen that implementing AI-based optimizations can enhance the efficiency of the process, decrease resource usage, and lower environmental effects, all while boosting biogas production and the efficient use of resources. The results have shown the possibility of the implementation of smart analytical systems for renewable energy production and sustainable waste management, through the optimization strategies based on collected data. The study also highlighted the importance of embedding predictive accuracy along with explainability for facilitating the decision-making on biomass utilization and bioenergy production by the stakeholders to understand the working of the system. The waste biomass utilization in the proposed framework yields valuable energy resources, in accordance with the aim of the circular bioeconomy which includes recycling of resources, protection of the environment and produced of renewable energy. Though these results are promising, future research will leverage larger and more diverse datasets, alternative sustainability metrics and more complex machine learning configurations to increase the predictive power and ease of use of the system. In addition, intelligent process control and real-time monitoring systems can be used to enhance the efficiency of AI systems in biogas production. The results indicate that the use of explainable artificial intelligence can effectively be a transparent, economical and scalable tool for optimizing the waste generation to energy conversion processes and sustainable bioenergy generation in modern frameworks of circular bioeconomy.

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