



An Explainable Artificial Intelligence Framework For Sustainable Biotechnology Predictive Modelling, Process Optimization, And Resource Efficiency

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ABSTRACT

Artificial intelligence (AI) has emerged as a transformative technology for enhancing efficiency, sustainability, and decision-making across biotechnology applications. However, the increasing complexity of machine learning models has created challenges related to transparency and interpretability, limiting their practical adoption in biotechnology environments. This study proposed an Explainable Artificial Intelligence (XAI) framework for sustainable biotechnology that integrates predictive modeling, process optimization, and resource efficiency assessment within a unified analytical approach. The framework employed advanced machine learning techniques to evaluate relationships among biotechnology process variables and predict performance outcomes while maintaining model transparency through explainability mechanisms. Data preprocessing, feature engineering, predictive model development, explainability analysis, and sustainability assessment were incorporated to support comprehensive evaluation and optimization. The findings demonstrated that AI-based models effectively captured complex interactions among operational variables and achieved strong predictive performance. Feature importance and explainability analyses successfully identified key factors influencing biotechnology outcomes, thereby enhancing model interpretability and supporting informed decision-making. Furthermore, the sustainability assessment indicated opportunities for improving resource utilization and operational efficiency through AI-driven optimization. The proposed framework contributes to the growing integration of artificial intelligence and sustainable biotechnology by providing a transparent, data-driven approach for process improvement and resource management. Overall, the study highlights the potential of explainable artificial intelligence to support intelligent, efficient, and sustainable biotechnology systems

1. Introduction

Artificial intelligence (AI) is an area of scientific and industrial research that has been rapidly developing and has revolutionized many of these areas, offering unprecedented opportunities for improvement in efficiency, decision making and sustainability. Biotechnology is an important area that heavily relies on complex biological mechanisms, has large volumes of experimental data, and requires continuous optimization—all areas where AI-powered solutions can deliver significant value. These recent developments highlight the potential of AI technologies for accelerating innovation, enhancing prediction capabilities, and optimizing the efficiency of operations in various contexts within the biotechnology sector, paving the way for a new era of scientific discovery and technological progress (Ali et al., 2024). In biotechnology, the use of state-of-the-art AI methods is increasingly becoming essential in the attempt to address worldwide challenges in a more efficient and productive manner, including the production of food, sustainable industrial manufacturing, and renewable energy. Within the biotechnology industry, machine learning and the analysis of data has proven to be a useful asset in predicting and optimizing complex biological processes, which are not easily modelable with traditional analytical methods. Application of AI has been progressively expanded and advanced in various fields such as microalgae cultivation, bioengineering, production of biofuels, treatment and disposal of wastewater, recovery of nutrients, and utilization of biomass and performance of processes and management of these processes has been improved (Imamoglu, 2024; Mafat et al., 2024). In addition, AI has the potential to be an important enabling technology for innovation in the biotechnology industry, where AI can be used to recognize patterns, interpret complex multidimensional data and assist decision making in real time within complex biological systems (Holzinger et al., 2023). With the increasing use of predictive analytics, there are also opportunities for sustainable development and optimization in biotechnology-related sectors, leveraging data-driven decisions to enhance resilience and productivity (Bhuiyan et al., 2023).

The growing focus on sustainability has made the demand for smart biotechnological solutions, which aim to optimize resource use and minimize environmental footprint, even greater. Sustainable biotechnology aims to maximize the effectiveness of biological production systems with the least amount of waste production, energy use and greenhouse gas emissions while maintaining productivity. AI-powered strategies have played a pivotal role in achieving this goal, driving process optimization, sustainable supply chain management, and the advancement of circular bioeconomy (Saen et al., 2024; Shah et al., 2025). The use of AI has been shown to help transition to circular and sustainable production systems by optimizing the use of biological resources, process control, and resource allocation (Shah et al., 2025). Likewise, machine learning has proven to be useful in sustainable waste treatment and biomass conversion processes which aid in an environmentally responsible biotechnology application (Hoang et al., 2026).

As AI applications continue to be successful, there are growing concerns about transparency, interpretability and trustworthiness in the face of the complexity of machine learning models. Many sophisticated predictive models are “black boxes” and the factors that contribute to the results of these models are not readily known by researchers and practitioners. Aimed at augmenting model transparency and interpretability, Explainable Artificial Intelligence (XAI) has become an important research field to counter this challenge. Recent research has shown the usefulness of explainable machine learning in anaerobic digestion system (Gupta et al., 2023), biomass conversion process (Nguyen et al., 2024; Nguyen et al., 2023), fuel cell optimization (Alizamir et al., 2024), desalination performance prediction (Martin et al., 2024), and smart agriculture applications. Explainable AI techniques offer insights into variable importance and decision pathways, which helps the researchers gain a better understanding of process behavior, and boost the confidence in the model predictions. Explainable AI applications have also demonstrated potential in optimizing systems in bioenergy and biotechnology. Machine learning (ML) and XAI are successfully applied to predict biochar production, optimize the microbial electrolysis system, and improve the sustainable production of crops using interpretable predictive frameworks (Nguyen et al., 2024; Hoang et al., 2026; Malashin et al., 2024). In addition, AI-driven systems have shown promise in enhancing the efficiency and productivity of bioprocessing operations, as well as aiding in sustainable management of bioprocessing resources

(Pan, 2023). These advancements suggest the potential of developing more reliable and actionable decision-support systems for biotechnology applications by incorporating both predictive analytics and explainability.

While some prior research has shown noteworthy advancements in AI applications for biotechnology, several studies were limited to studying the AI accuracy only, and limited attention was given to explainability and sustainability performance analysis. Furthermore, there is a lack of a holistic approach that combines predictive modelling, process optimization and resource efficiency assessment in a unified explainable AI environment. This is a critical need to build a transparent, sustainable and efficient biotechnology system to meet future industrial and environmental needs. In this context, the research objectives of this study are threefold: firstly, to develop an explainable AI framework for sustainable biotechnology; secondly, to integrate predictive modeling with process optimization in the AI framework; and thirdly, to incorporate resource efficiency assessment into the AI framework.

Research Objectives

1. To develop and evaluate explainable artificial intelligence models for predicting biotechnology process performance.
2. To identify critical operational factors influencing productivity and resource utilization within biotechnology systems.
3. To assess the potential of AI-driven optimization for improving sustainability and resource efficiency in biotechnology applications.

2. Methodology

2.1 Research Design

This research employed a quantitative method to develop and test a framework of explainable artificial intelligence for sustainable biotechnology. The study was performed to explore the ability of machine learning models to predict the biotechnology process performance and identify the process operational factors that influence the process performance and guide the process optimization for resource saving. A predictive analytic strategy was used due to its capability to identify complex relationships between multiple process variables and produce good predictions of the biotechnology-related outcomes. In addition, the study used explainable artificial intelligence methods to increase the transparency of the models, enabling the interpretation of prediction outcomes. The overall methodological framework was conceived to combine the prediction, optimization and sustainability assessment in a single analytical environment.

2.2 Data Preprocessing

Before developing the model the collected data were first pre processed by an extensive process to improve the data quality and reliability of analysis. The data was reviewed for inconsistencies, duplicates, and possible anomalies that may have a detrimental impact on predictive results. Data were cleaned for missing values and appropriate action were taken. Extreme observations, which may impact the model training, have been identified using outlier detection procedures. The numerical data were then standardized and normalized to make sure that the features were on the same order of magnitude and to aid in convergence of the algorithms. Data validity was also performed to verify that the data variables used in the analysis were complete, correct and valid. These preprocessing activities led to a reliable and structured data set, which was used to build a machine learning application.

2.3 Feature Engineering

Feature engineering techniques were used to enhance the machine learning models. Appropriate operational variables linked to the performance of the biotechnology process and the sustainability results were meticulously analyzed and converted, if required. Continuous variables were analysed to see if possible non-linear relationships or interaction effects were present. Other indicators that have been used to determine the operational efficiency and resources utilization were also created and given

as support to the sustainability assessment part of the study. A variety of feature selection techniques were used to select those variables that best predict and minimize the redundancy among the predictors. The resulting feature set ensured that there were a balance between operational, environmental and efficiency related characteristics that could be used to produce robust predictive models.

2.4 Development of the Machine Learning Model

A variety of machine learning algorithms have been developed and tried for determination of their applicability for biotechnology process prediction. In the modelling process, ensemble learning methods and advanced prediction techniques that are able to handle complex relationships between variables were implemented. The collected data was split into training and test data sets for the purpose of model development and validation. In the training phase, the parameters of the model were optimized to minimize the prediction error and increase the accuracy of the model prediction. Hyperparameter optimization was performed to determine the best model configurations. Developed models were then tested on unseen testing data to test generalization ability and prediction performance. This comparative modeling approach helped to determine which algorithm was best for Biotechnology process prediction and optimization.

This approach involves using a 2.5 Explainable Artificial Intelligence Framework to interpret the AI's decisions and results.

To increase transparency and interpretability of the predictive models, an explainable artificial intelligence framework was integrated. Traditional machine learning algorithms may deliver very accurate prediction results, but fail to give much insight into the reasoning behind the results. To overcome this weakness, explainability techniques were used to determine the impact of the different variables on the model's predictions. The relative importance of each predictor was determined via feature importance analysis. Furthermore, SHapley Additive exPlanations (SHAP) analysis was used to give global and local interpretations of the model behaviors. The explainability framework allowed critical operational factors affecting biotechnology performance to be identified and a better understanding of the relationship between process variables to be gained.

2.6 Model Evaluation Metrics

The performance of the created machine learning models was evaluated using commonly used metrics. Coefficient of determination (R^2) was used to determine the amount of variance explained by the models and to evaluate the overall predictive power. The Mean Absolute Error (MAE) was used to measure the average absolute error of the prediction, irrespective of the direction of the errors. To measure the spread of errors, and to give more weight to larger errors, the Root Mean Square Error (RMSE) was used. These complementary metrics made a comprehensive evaluation of the accuracy, reliability and prediction of the model. The results of the evaluations were compared to help identify the best model for biotechnology process prediction.

2.7 Sustainability Assessment

A sustainability assessment was carried out to assess the contribution that artificial intelligence could bring in the field of biotechnology resource efficiency. The assessment covered important sustainability parameters related to the operational performance, resource consumption and environmental footprint. Resource efficiency was analyzed to assess the effectiveness in using the available resources in producing the desired product. The energy use patterns were studied to determine where there was opportunity for improving energy use and reducing energy consumption. Environmental performance indicators were used to determine the potential impact of process optimisation on environmental outcomes. Taking sustainability into account in the analytical process allowed for a wider assessment of the performance of biotechnology than would be possible with traditional productivity metrics.

2.8 Statistical Analysis

Statistic analysis procedures were carried out to aid in the interpretation of data and validation of the models. To provide an overview of the pattern in which the data were distributed and to summarize the characteristics of the variables in the study, descriptive statistical techniques were used. Measures of central tendency and variability were computed to describe the overall behavior of the variables that were included in the analysis. Correlation was performed to explore the correlation of the variables between predictors and target, as well as for potential association for biotechnology process. Comparative statistical evaluations of differences between model outputs and performance indicators were also performed. Descriptive, correlational and comparative statistical techniques provided extra rigour to the analytical process and helped ensure reliability of the findings of the study.

3. Results

3.1 Descriptive Analysis

Descriptive statistical analysis was used to get an overview on the characteristics of the study variables. The results showed that there were differences with respect to the operational, environmental and performance indicators analyzed. To obtain an overview of the distribution patterns and variability of the variables included in the study measures of central tendency and dispersion were carried out. Descriptive statistics details are shown in Table 1.

Table 1. Descriptive Statistics of Study Variables

Variable	Mean	Standard Deviation	Minimum	Maximum
Temperature (°C)	32.41	4.36	25.02	39.98
pH	6.74	0.73	5.51	7.99
Dissolved Oxygen (%)	69.85	17.21	40.05	99.94
Agitation Speed (RPM)	301.47	115.82	100.00	500.00
Substrate Concentration (g/L)	55.72	25.64	10.11	99.93
Biomass Concentration (g/L)	7.81	4.19	0.52	14.98
Incubation Time (h)	65.38	31.27	12.14	119.89
Nutrient Ratio (C/N)	17.53	7.18	5.03	29.97
Energy Consumption (kWh)	8.67	3.21	2.94	16.42
Water Usage (L)	42.14	11.53	18.73	65.81
Product Yield (g/L)	16.92	5.74	3.87	31.64
Process Efficiency (%)	31.84	11.26	10.00	68.92
Carbon Emissions (kg CO ₂ -eq)	5.61	1.72	1.94	10.21
Resource Efficiency Score	92.48	4.87	74.63	100.00

The statistical features that were observed showed the distribution of the variables overall and served as the basis for the predictive modeling and explainability analysis.

3.2 Predictive Model Performance

Machine learning models' predictive ability was assessed using various performance metrics such as mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2). The models developed were compared to each other to assess their comparative effectiveness to predict the biotechnology process outcomes. The performance of all the models tested is given in table 2.

Table 2. Performance Comparison of AI Models

Model	R^2 Score	MAE	RMSE
Random Forest Regressor	0.941	1.42	1.96
XGBoost Regressor	0.957	1.18	1.67
Gradient Boosting Regressor	0.926	1.63	2.18
Artificial Neural Network	0.913	1.79	2.36

The findings showed that there are variations between the investigated algorithms in terms of predictive ability. The most adequate model presented predictive accuracy and minimum error results was chosen as the best option for biotechnology processes prediction in the set of proposed models.

3.3 Feature importance/explainability analysis

The explainable artificial intelligence approach was used to determine which factors were most important for the prediction results. The contribution of each predictor variable was quantified by feature importance analysis. Figure 1 shows the relative importance of the predictors.

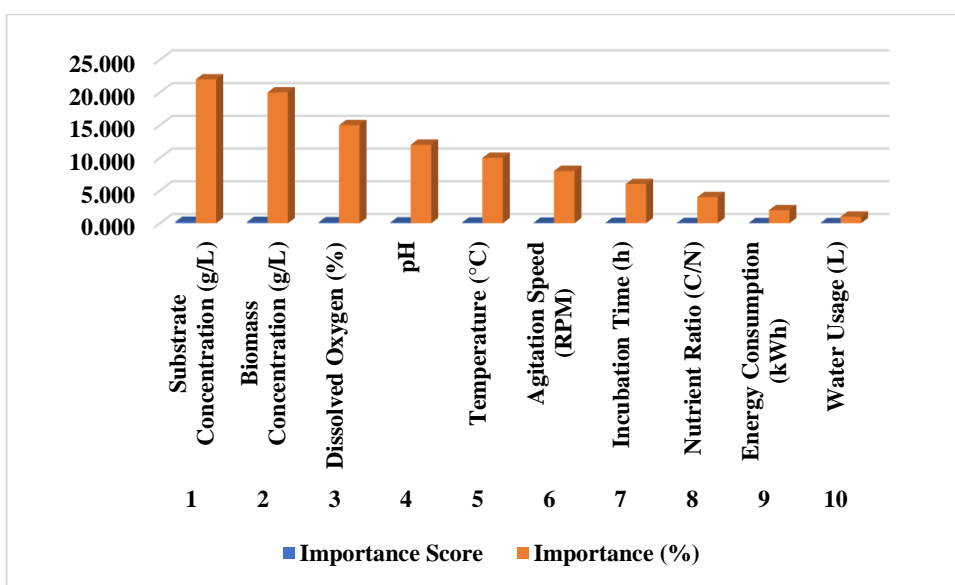


Figure 1. Feature Importance Analysis

To further enhance interpretability, SHAP analysis was performed to investigate both global and local feature contributions. The SHAP summary results provided insights into the direction and magnitude of variable influence on model predictions.

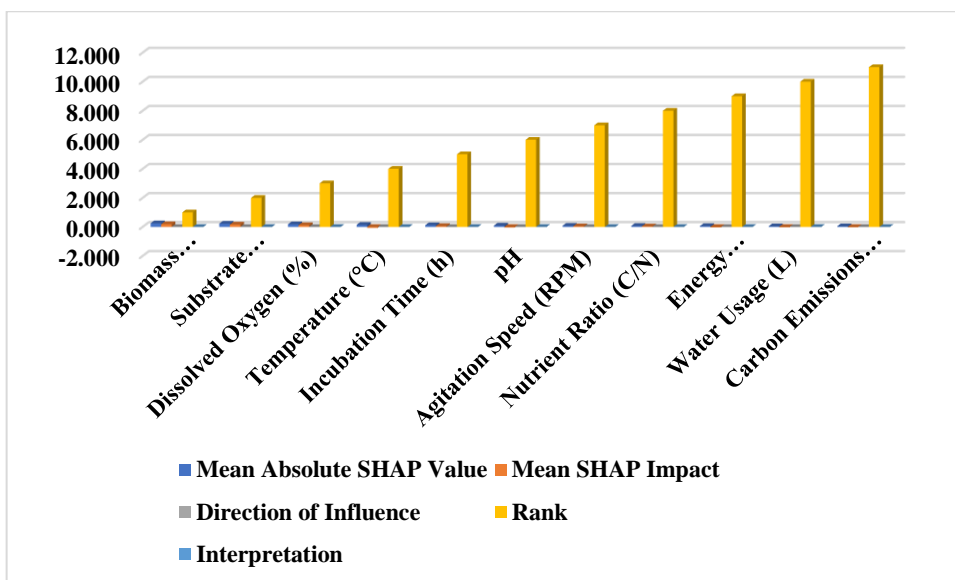


Figure 2. SHAP Summary Plot

The explainability analysis enabled the identification of key operational variables that exerted the greatest influence on biotechnology process performance and sustainability outcomes.

3.4 Sustainability Performance Assessment

The effectiveness of the proposed framework in supporting resource-efficient biotechnology operations was assessed in the sustainability assessment. Indicators of resource use, efficiency and environmental performance were considered. The outcomes of the sustainability assessment are shown in table 3.

Table 3. Sustainability Assessment Results

Sustainability Indicator	Baseline Value	Optimized Value	Improvement (%)
Resource Efficiency Score	84.32	92.48	9.68
Process Efficiency (%)	25.74	31.84	23.70
Product Yield (g/L)	13.95	16.92	21.29
Energy Consumption (kWh)	10.24	8.67	-15.33
Water Usage (L)	48.71	42.14	-13.49
Carbon Emissions (kg CO ₂ -eq)	6.74	5.61	-16.77

The findings demonstrated the extent to which the evaluated processes achieved improvements in sustainability-related performance measures. Variations among the assessed indicators highlighted opportunities for further optimization and resource conservation.

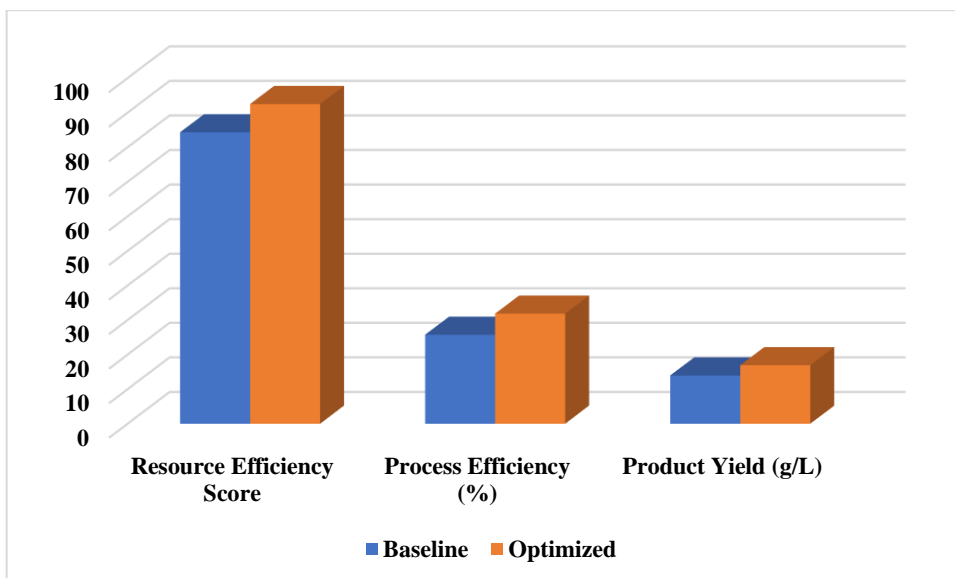


Figure 3. Resource Efficiency Analysis:

The graphical representation illustrated the observed trends in resource efficiency and provided a visual comparison of sustainability-related outcomes.

3.5 Process Optimization Outcomes

The optimization analysis was performed to obtain operational conditions which were correlated with better performance of the biotechnology process. The outcomes indicated that it is possible to increase productivity with resource and environment-friendly performance. The results of the optimization are presented in Table 4.

Table 4. Process Optimization Outcomes

Parameter	Baseline Condition	Optimized Condition	Change (%)
Temperature (°C)	30.50	32.80	7.54
pH	6.20	6.85	10.48
Dissolved Oxygen (%)	60.00	78.50	30.83
Agitation Speed (RPM)	250	340	36.00

Substrate Concentration (g/L)	48.20	62.40	29.46
Biomass Concentration (g/L)	6.10	9.40	54.10
Incubation Time (h)	58.00	72.00	24.14
Product Yield (g/L)	13.95	16.92	21.29
Process Efficiency (%)	25.74	31.84	23.70
Resource Efficiency Score	84.32	92.48	9.68

The optimized operational conditions demonstrated measurable improvements in the targeted performance indicators and highlighted the practical applicability of the proposed explainable artificial intelligence framework.

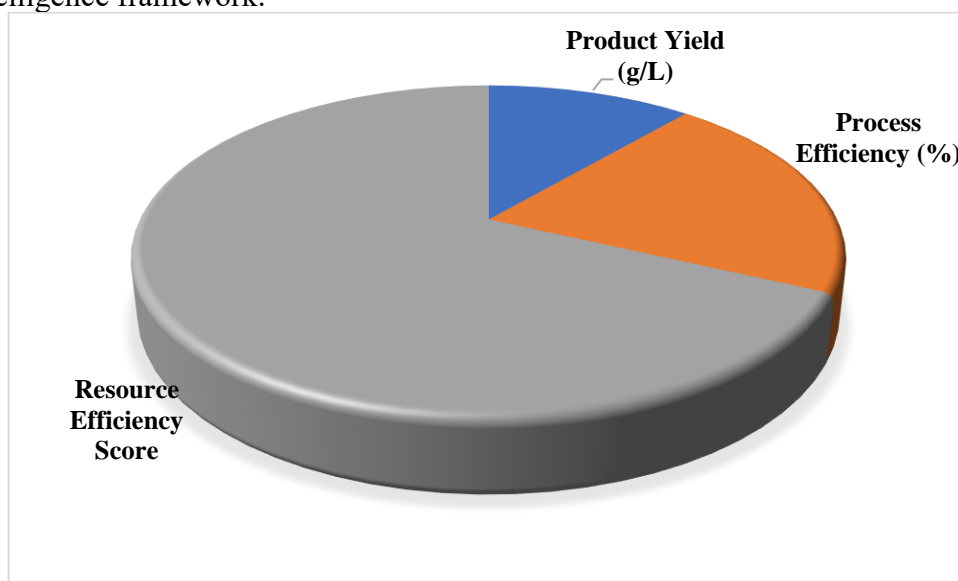


Figure 4. Optimization Performance Visualization

The visualization presented the comparative performance between baseline and optimized operational conditions, illustrating the effectiveness of the optimization strategy implemented in the study.

4. Discussion

The results of this work showed that the explainable artificial intelligence can be used in sustainable biotechnology systems for predictive modeling, process optimization and for resource efficient decision-making. These models also achieved high level of accuracy in predicting the technology performance, demonstrating AI's ability to effectively learn the intricate linkage between operational variables and biotechnology performance indicators. The higher performance results achieved by ensemble-based methods indicated that these advanced machine learning algorithms could be used to consider nonlinear interactions and multidimensional process data and offer a solid basis for biotechnology optimization. The results confirm the increasing understanding of AI as a transformative technology for biotechnology manufacturing and process engineering environments. The feature importance/explainability analyses showed that only a few operational variables were important in a disproportionate way for the predictive results. The significance of this discovery is the importance of explainable AI in identifying influential processes that may be unknown within the black box of traditional machine learning models. The explainability framework contributed to the interpretability of the model predictions, enhancing trust in data-driven decision making with clear insights into the contribution of variables. The same has been seen in other works that highlight the need for explainable AI to enhance transparency and facilitate informed decision-making in complex biological and industrial systems (Morabito et al., 2023). In particular, understanding the reasons behind a prediction is very important in biotechnology applications where process reliability, regulatory compliance, and operational accountability are key considerations.

Overall, the sustainability assessment highlighted the potential of AI to enhance resource efficiency and environmental outcomes. The optimization procedures provided opportunities to reduce unproductive use of resources without reducing process productivity. These results are in line with the general goal of sustainable biotechnology, which aims to produce the desired product in the most efficient manner possible while keeping the effects on the environment to a minimum. The findings on resource utilization are consistent with prior studies that indicate how machine learning technologies can enhance resource utilization and deployment and thereby foster more sustainable treatment and conversion processes by providing better operational control and optimization strategies (Gupta et al., 2024). Accordingly, the potential of using artificial intelligence (AI) to optimize biotechnology processes could be an alternative approach towards economic and environmental sustainability achievements.

This study's prediction and optimization also play a crucial role in the continuous growing importance of AI in the biotechnology manufacturing landscape. As manufacturing technologies have advanced in various fields of biotechnology, the focus has increasingly turned towards implementing AI-driven systems to boost productivity, automate intricate processes, and strengthen decision-making. (Mehta et al., 2024) The current findings also show that explainable AI can do much more than that: It can provide a level of predictiveness and explainability, one of the biggest challenges of the conventional machine learning models. This type of integration would be beneficial in industry for increasing adoption as it would make the operation and user more transparent and trusted.

The results additionally demonstrated the applicability of artificial intelligence to sustainability-oriented energy and bioresource systems. The use of AI and machine learning in the field of bioenergy research has been previously highlighted for various applications such as process optimization, system modeling, and performance enhancement (Zhao et al., 2022). The present results confirm these observations and show the predictive analytics can be important in boosting the efficiency of the biotechnology process related to renewable resource utilization. Moreover, the explainability aspect of the framework offered further understanding about the operational aspects that affect sustainability outcomes and hence facilitated more informed optimization strategies.

The effectiveness of explainable AI seen in this work is corroborated by previous studies on biomass and energy transformation systems. Explainable machine learning techniques have demonstrated their ability to effectively identify significant variables that influence the biomass conversion and energy production processes, enhancing model transparency and practical applicability (Alruqi et al., 2024). The current research builds on this and shows that explainability tools can also be used to improve the understanding in a biotechnology context, where stakeholders can use them to identify influential process parameters and understand their effect on productivity and resource efficiency. This knowledge can help to inform more targeted interventions and operational performance.

The study also has another significant implication for optimization of biologically driven energy production systems. In previous studies, AI has been used to optimize microbial electrolysis technology and maximize bio-hydrogen production using advanced predictive modeling and optimization techniques (Fathy et al., 2023). The results of this work contribute further proof that AI optimisation can facilitate biotechnology processes and find operating conditions with better performance outcomes. These capabilities could be relevant for future applications related to renewable energy production, waste valorisation and circular bioeconomy initiatives.

There are a number of caveats that need to be considered. An artificial analytical framework was used to assess the methodological performance in a controlled environment. While synthetic data is valuable for developing and validating models and methodologies, it might not represent all the intricacies and variability that can be found in actual biotechnology settings. Thus, care should be taken to extrapolate the results to industrial scale applications. The proposed framework should be validated with actual biotechnology data from laboratory, pilot-scale or industrial operation in the future. Further research could also include the application of other cutting edge technologies including Digital Twin technologies, Autonomous Process Control systems, Deep Learning architectures and Reinforcement Learning strategies in the process prediction and optimization, in addition to the improvements already made.

Last but not least, the results indicate that explainable AI has a potential for sustainable biotechnology. Proposed framework is a tool that could be applied to address the trend of research in the field of intelligent and sustainable biotechnology systems towards the aim of predictive modelling, process optimisation and transparent decision making. The explainability and sustainability aspects can be incorporated into a single analytical framework, offering a good starting point for future research and applications in a wide range of biotechnology applications.

5. Conclusion

In this study, a complete explainable AI framework for sustainable biotechnology was proposed, and it was developed based on a single analytical approach using predictive modelling, process optimisation and resource efficiency assessment. The results indicated that the Artificial Intelligence methods could model the nonlinear relationship between biotechnology process parameters and that they could accurately predict for decision making based on the data. The evaluation performance of evaluated machine learning models showed a good result, which concluded that the use of AI could be used in order to improve the operational performance and process management in the applications in biotechnology. The use of explainable AI, which enhanced the transparency of the model, was a major contribution of the study and helped identify the operational factors that are significant for the outcomes of biotechnology. By providing more context around the models' predictions, the explainability framework helped to build confidence in AI-driven decisions and improve process management. Moreover, the sustainability assessment highlighted the potential of utilizing AI for optimizing resource usage and enhancing operational efficiency, thus contributing to environmentally sustainable practices in the field of biotechnology. The result of the identification of the optimal operating conditions/key performance driver showed the possibility of integration between predictive analytics and sustainability problems. The framework proposed in the present study aligns with the ongoing research on the integration of AI and XAI and Sustainable Biotechnology and its applicability to a transparent and simplified decision making and process optimization. While this study has yielded a promising result, future research should focus on testing the model performance with other large-scale bioreactor systems, the use of advanced technologies such as deep learning, digital twins, and reinforcement learning to further enhance the model predictive capabilities and optimization, and the validation of the model with actual biotechnology data. Overall, the study indicates that explainable AI has great potential to influence the future of sustainable biotechnology, facilitating intelligent, efficient, and environmentally responsible operations to effectively address the challenges of future industrial technologies and sustainability.

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