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Integration of Mathematical Modeling and Artificial Intelligence to Predict Thermal Conditions and Optimize the Operation of Biogas Plants

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Abstract

Modern biogas plants face a number of challenges related to precise control of thermal conditions, which significantly affect the stability of processes and the overall efficiency of energy production. The complexity lies in the nonlinear and dynamic nature of biochemical reactions occurring under anaerobic conditions, as well as in a large number of factors affecting heat transfer inside the reactor. In this regard, there is a need to develop adaptive and highly accurate models capable of predicting thermal processes and optimizing the operation of biogas systems. In this study, we propose a hybrid modeling framework that integrates physics-based mathematical models with machine learning algorithms, enabling real-time prediction and adaptive control of thermal processes. Unlike prior models focused solely on thermodynamics or empirical learning, our approach synergistically combines mechanistic equations (*e.g.*, Navier-Stokes, reaction kinetics) with artificial intelligence (AI) techniques (*e.g.*, neural networks, gradient boosting), yielding improved accuracy, lower energy loss, and higher biogas output. The results obtained demonstrate an increase in the plant's productivity, a decrease in energy losses and an improvement in environmental indicators, which makes this model a promising tool for managing sustainable energy systems.

Keywords: Biogas plants; Mathematical model; Optimization; Artificial intelligence; Machine learning.

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1. Introduction

In the context of the global shift to renewable energy sources, biogas planting is becoming a more important part of energy infrastructure. Biogas planting enables recycled organic wastes, converting them into useful energy and concurrently addressing waste disposal issues. However, the efficient operation of biogas plants requires the accurate management of thermal processes, a challenging task due to the dynamism and non-linearity of the process.[1] Developing methods is crucial for enhancing the efficiency of the biogas plant process, as it enables precisely predicting the thermal regime and optimizing the planting process. Within this scope mathematical modeling constitutes a powerful tool, which can be applied to analyze thermal processes and develop management strategies. In recent years, artificial intelligence methods, including machine learning and neural networks proved to be effective in tackling sophisticated prediction activities and optimization. The study aims to develop and analyze mathematical models for predicting thermal regimes and enhancing biogas plant operations using artificial intelligence methods. During the study, the authors explore the main principles of simulation of thermal processes in biogas plants and approaches to applying artificial intelligence methods to enhance the accuracy of prediction and management efficiency.[2] The present study holds significant theoretical and practical value. On the one hand, it contributes to refining the theoretical framework of modeling and managing thermal processes in biogas plants.[3] On the other hand, study results can be directly employed in design

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applications and operating the biogas planting that allows to enhance efficiency, reduce maintenance costs, and make a contribution to developing sustainable energy.

The contemporary advancement of technologies in renewable energy calls for precise and effective methods of management and process optimization. Biogas plant, converting organic wastes into biogas, is an essential component of sustainable energy. However, precise methods of predicting and thermal regime controlling are necessary for ensuring its effective functioning. Regarding this matter, implementing mathematical models and artificial intelligence is more relevant.[4] Research in biogas plants and their optimization is actively developing in the light of crucial need for adopting renewable energy sources. One important part of the process is a precise prediction of the thermal regime while planting, which directly impacts its efficiency. In recent years, mathematical models and artificial intelligence methods have become the key tools in tackling issues in terms of thermal process management in biogas plants.

The mathematical modeling of thermal processes in biogas plants has a well–established history. Initial studies, the research were directed towards creating a basic model, that described thermal and chemical processes within the biogas reactors.[3] These models were the foundation for further development and improvement. Contemporary research focuses on more complex and precise models. For example, there were proposed models, aimed at organic material decomposition kinetics and factors affecting thermal regime. The models enable more accurate prediction of biogas plant behavior in various operating conditions. Advancements in AI technologies have enabled substantial enhancements in the accuracy of mathematical models. Machine learning methods and neural networks are being widely applied in foreseeing thermal regimes. The research displays the successful implementation of neural networks for predicting temperatures and other key aspects of biogas plants.

Integrating AI with traditional mathematical models is crucial.[5] As the research shows, combining machine learning techniques with physics-based models facilitates achieving high accuracy of prediction and improves the thermal process management.[6] Improving the operation of biogas plants is key to enhancing their efficiency. Studies in the matter are directed towards developing algorithms, that allow to reduce energy cost and maximize biogas outputs. Demonstrate the successful implementation of optimization methods based on AI to manage the thermal processes and enhance the biogas plant.[1] Applying the developed models and algorithms in real-world scenarios reveals significant improvements in the efficiency of biogas plants. The research proves that employing AI in thermal process management can reduce operating costs and increase energy output. Further research perspectives include creating more comprehensive and adaptive models that can consider a wide range of factors affecting the biogas plant operation. Moreover, integrating AI with cutting–edge technologies such as the Internet of Things (IoT) and Big Data promise considerable improvement in management and biogas system optimization.[7,8] As the literature review reveals, mathematical models and artificial intelligence methods play a key role in the prediction and optimization of thermal regimes in biogas plants. Developing these methods facilitates to improvement of the efficiency of biogas plants significantly, which is a main step towards sustainable energy.[9]

Over the past two years, there has been significant progress in the use of artificial intelligence methods to optimize the operation of biogas plants. An innovative approach using deep neural networks to predict biogas yield was proposed in the work.[10] The complexity of the issues of process optimization in biogas plants was also confirmed in the publication,[11] where the researchers used heterogeneous model integration methods to improve the accuracy of forecasts. Additional confirmation of the importance of such approaches can be found in the publication where machine learning algorithms were used to develop sensors that monitor the ratio of volatile fatty acids to alkalinity.[12] The studies focused on optimizing the design and management solutions of biogas plants using machine learning algorithms, which confirms the effectiveness of such approaches in various operating scenarios.[13] Thus, unlike most existing works aimed exclusively at predicting biogas production, this study is distinguished by the complexity of its approach. The integration of physical and mathematical modeling with artificial intelligence methods allows not only to accurately predict the thermal regime, but also to take into account the influence of the heat balance, hydrodynamics and mass of matter. This approach enables more adaptive process control and is an important step towards improving the efficiency and sustainability of biogas systems.

While earlier research has applied either physics-based models or artificial intelligence separately to manage thermal regimes in biogas plants, our work is distinguished by its integrative, dual-layered approach. We embed AI algorithms into the structure of a mechanistic thermal model, allowing for adaptive learning from sensor data while preserving physical interpretability. This hybridization enables the system allows respond to environmental and operational changes in real time, which traditional models lack. Furthermore, our approach addresses multivariate optimization goals—such as maximizing methane yield while minimizing thermal energy loss—through evolutionary computation, which has rarely been done in prior studies.

2. Experimental section

2.1 Material preparation

A complex approach with the following steps and methods was selected to investigate the thermal regime prediction models and functioning biogas planting.

1. Data collection and planting parameters analysis. Before the study, data was collected regarding the composition of raw materials, technical parameters, and external parameters in operating biogas plants.[14]
2. Developing mathematical models. Based on the collected data, a mathematical model was developed. It considered biochemical reactions within the reactor vessel, thermal flow within the system, and energy loss.
3. Model integration with software. The model was implemented by using software, computational modeling in Python leveraging libraries, for solving differential equations and optimization.[15]
4. Model validation. Mathematical model validation was conducted based on the experimental data obtained from real-time biogas production. It includes comparing predicting thermal characteristics with actual metrics.[16]
5. Optimization and analysis: the model was used for optimizing the performance of planting such as minimizing energy loss, or maximizing biogas production. Analysis was conducted on the effects of various factors on planting efficiency.

This approach enables one to gain a thorough understanding of the process, occurring during biogas planting, and design strategies for improving its performance and sustainability in the long run.

The key components including thermal balance, biochemical reaction, hydrodynamics, and flow mass should be considered during developing mathematical models for predicting the thermal regime and functioning of the biogas plant. The model considers all the parameters for precise prediction.[17]

The data obtained from operating biogas plants was employed to develop and analyze the mathematical models. As an external data was taken:

- Temperature indicators: measurements of temperature within the reactor, environment, and temperature of supplied raw material.
- Raw material characteristics: the content of organic waste, moisture, carbon, and nitrogen content.
- Operational parameters: loading volume, retention time, mixing speed, and pressure.
- Industrial parameters: biogas output, methane and carbon dioxide content, and energy efficiency.

Moreover, a differential equation system was used to design the thermal regimes for biogas plants. The main thermal and chemical progress were described in Eq. (1):[3,4]

$$\frac{dT}{dt} = f(T, C, P, \dots) \tag{1}$$

where T is the temperature, C is the concentration of reagents, P is the pressure, and so on.

A basic model was designed using equations for heat transfer and chemical reaction kinetics, considering: convection and heat conductivity; exothermic and endothermic reactions; effects of mixing and raw materials supplied.

In this study, a neural network is used to approximate the biochemical processes in a biogas plant. The architecture includes two hidden layers of 64 neurons each with ReLU activation function. Training was performed using Adam optimizer and MSE loss function. A gradient bousting algorithm was also applied to compare the approximation accuracy. Both models showed high efficiency with low consumption of computational resources.

Description of the neural network architecture used in the study: Input layer: 1 neuron - takes time t as the only input parameter. Hidden layers, first hidden layer: 64 neurons, activation function is ReLU. second hidden layer: 64 neurons, activation function is ReLU. Output layer: 4 neurons - each corresponding to output concentration values: S_h (hydrolyzable substrates), S_a (volatile fatty acids), S_ace (acetate), S_CH4 (methane). Activation function is linear. Loss function-Mean Squared Error (MSE), optimizer-Adam, number of epochs-100, batch size-10.

The model's adequacy was assessed using actual data gathered from the biogas plant. Additionally, the model was calibrated and verified by adapting statistical methods, such as coefficient of determination and mean squared error (MSE). Machine learning methods, particularly neural networks, and gradient boosting algorithms were employed to predict the thermal regime and optimization of the Biogas production process. A neural network is a multilayer perceptron model, trained using data on thermal and production parameters, while gradient boosting was employed to enhance the accuracy of predicting and the control settings. Similarly, a hybrid model was implemented to enhance the accuracy and reliability of prediction. Hybrid model integrated mathematical modeling grounded in physical principles and machine learning algorithms. The obtained data was clustered into training and testing sets to develop and evaluate the models.[18]

Optimization of the operation of a biogas plant is considered as a multi-criteria optimization problem, in which the aim is to simultaneously minimize operating costs and maximize energy production. The issues were addressed using evolutionary algorithms and global optimization methods, which included genetic algorithms and particle swarm optimization (PSO). The designed model and algorithms were coded in Python, as well as in machine learning libraries, namely TensorFlow and Scikit-learn.[19] The testing was conducted using actual data from a biogas plant to evaluate the efficiency of the proposed methods.[20,21]

The materials and methods presented propose an integrated approach for studying and optimizing the thermal regime of biogas plants. Developing and integrating mathematical models with artificial intelligent methods facilitate a substantial enhancement in prediction accuracy and efficiency of the biogas planting process.

2.2 Thermal balance

The equation Eq. (2) describes the total energy change in the system as a balance between external heat input, biochemical heat generation, and losses to the environment. The heat generation term Q_{bio} stems from the exothermic nature of anaerobic digestion, particularly methanogenesis, which releases energy. Literature reports the heat of reaction for acetate-to-methane conversion at approx. –135 kJ/mol CH_4,[22] which supports the magnitude and direction of Q_{bio}. The loss term is modeled based on Newton's law of cooling: $UA(T_{reactor} - T_{ambient} = Q_{loss}$, where U is the global heat transfer coefficient, estimated from experimental calibration. The main equation of thermal balance is formulated.[22]

$$Q_{in} + Q_{out} + Q_{gen} = Q_{stored} \tag{2}$$

where Q_{in} is the thermal energy, entering the system (through bioreactor heating), Q_{out} is the thermal energy, exiting the system (through heat exchanger); Q_{gen} is the thermal energy, generated as a result of biochemical reactions; Q_{stored} is the changes in stored thermal energy in the system.

Table 1 summarizes the main model parameters, their symbols, typical values or ranges, and sources. Parameters were selected based on established literature or calibrated using experimental data. This supports the theoretical basis and reliability of the proposed model.

2.3 Biochemical reactions

Kinetics equation Eq. (3) can be used for modeling biochemical reactions:[4]

$$\frac{dC}{dt} = \mu_{max} \frac{S}{K_S + S} C \tag{3}$$

where C is the biomass concentration; μ_{max} is the maximum rate of microbial growth; S is the substrate concentration (organic substance); K_S is the saturation constant (half saturation).

2.4 Hydrodynamics

Navier – Strokes equation Eq. (4) was used to describe the flow and blending within the bioreactor:[23]

$$\rho\left(\frac{\partial}{\partial t} + (u \cdot \Delta)u\right) = -\Delta p + \mu\Delta^2 u + f \tag{4}$$

where ρ is the liquid density; u is the flow velocity vector; p is the pressure; μ is the dynamic viscosity; f is the volumetric force.

2.5 Mass balance

The mass of circulation and substrates can be described using the continuity equation Eq. (5):[16]

$$\frac{dM}{dt} = \sum Q_{in} + \sum Q_{out} + R \tag{5}$$

where M is the substance mass (substrates, biomass and *etc*.); Q_{in} is the input of mass flow; Q_{out} is the output of mass flow; R is the generation speed or substance consumption as a result of biochemical. reactions.

2.6 Energy balance

Energy balance can encompass calculations Eq. (6) for the entire system:[22]

$$E_{in} - E_{out} + E_{gen} = E_{stored} \tag{6}$$

where E_{in} is the energy input into the system; E_{out} is the energy output from the system; E_{gen} is the energy generated

Table 1: Key parameters used in the mathematical and AI-based model for biogas plant optimization.

Parameter	Symbol	Value/Range
Max microbial growth rate	μ_{max}	0.3–0.7 h^{-1}
Half-saturation constant	K_s	0.1–1.0 g/L
Heat of methanogenesis	ΔH_{meth}	–135 kJ/mol
Heat transfer coefficient	U	30–50 $W/m^2 \cdot K$
Bioreactor volume	V	10–100 m^3
Density of fluid	ρ	1000 kg/m^3

by the system; E_{stored} is the changes in stored energy in the system.

These equations can be used as a foundation for creating mathematical models. Specific parameter values and detailed equations will depend on the characteristics of a biogas plant, operation conditions, and modeling targets.[23]

During the development of kinetics equations in biochemical reactions, where the main processes of methanogenesis are considered, it is important to consider several main stages, namely hydrolysis, acidogenesis, acetogenesis, and methanogenesis. The stages occur within anaerobic settings in bioreactors.[24]

2.7 Hydrolysis

Hydrolysis is a decomposition process of complex organic compounds (carbohydrates, proteins, and lipids) to simpler molecules (and fatty acids). Eq. (7) for hydrolysis can be formulated:[4,25]

$$\frac{dS_h}{dt} = k_h S_h \tag{7}$$

where S_h is the concentration of hydrolyzable substrates, k_h is the hydrolysis rate constant.

2.8 Acidogenesis

Acidogenesis is a process where simple molecules (monosaccharides, amino acids) are converted into volatile fatty acids, hydrogen, and carbon dioxide. The acidogenesis describing equation Eq. (8) is illustrated:[4,26]

$$\frac{dS_a}{dt} = k_a S_h - k_b S_a \tag{8}$$

where S_a is the concentration of acidogenizable substrates; k_a is the acidogenesis rate constant, k_b is the rate constant for the consumption of acidogenizable substrates occurs in the subsequent step.

2.9 Acetogenesis

Acetogenesis is a process of converting volatile fatty acids and alcohol into acetate, hydrogen, and carbon dioxide. The acetogenesis process can be formulated Eq. (9) as follows:[4,25]

$$\frac{dS_{ace}}{dt} = k_c S_a - k_d S_{ace} \tag{9}$$

where S_{ace} is the concentration of acetate; k_c is the acetogenesis rate constant; k_d is the rate constant for the consumption of acetate in the subsequent step.

2.10 Methanogenesis

Methanogenesis is the final step where acetate and hydrogen turn into methane and carbon dioxide. The following equation Eq. (10) applies to methanogenesis:[14]

$$\frac{dS_{CH_4}}{dt} = k_e S_{ace} - k_f S_H \tag{10}$$

where S_{CH4} is the methane concentration; S_H is the hydrogen concentration; k_e is the rate constant of methanogenesis from acetate; k_f is the rate constant of methanogenesis from hydrogen.

Complex equations. By combining all stages of Eqs. (7)-(10), a differential equation system can be made, where all processes of methanogenesis presented Eq. (11):

$$\begin{cases} \frac{dS_h}{dt} = -k_h S_h \\ \frac{dS_a}{dt} = k_h S_h - k_a S_a \\ \frac{dS_{ace}}{dt} = k_h S_h - k_a S_{ace} \\ \frac{dS_{CH_4}}{dt} = k_c S_{ace} - k_f S_H \end{cases} \tag{11}$$

where all concentration and constant rates align with the corresponding stages and intermediate products.[24]

3. Results

The study will culminate in a complex mathematical model, which allows us to predict accurately the thermal regime of biogas plants. The developed model and implementation of AI technologies will facilitate: increase the efficiency of the biogas plant; reduction of energy cost on maintaining an optimal thermal regime; increased biogas output by optimizing the process parameters.

Integrating mathematical models with artificial intelligence in thermal process management during biogas planting provides new prospects for improving efficiency and reliability. Developing and implementing such management systems will foster the development of renewable energy sources and ensure a long–term sustainable energy future.[27]

The equations system outlines the kinetics of the main biochemical processes that are related to methane generation in biogas plants. Designation of constant rates k_h, k_a, k_c, k_d, k_e, k_f was defined experimentally, depending on the specifics of the biogas plant under consideration.

The data in Figs. 1 and 4 was obtained experimentally. Upon resolving the system of differential equations, graphical representations were generated to illustrate theoretical, approximate, and experimental data. Moreover, the following results of graphics were obtained after solving a system of differential equations and then creating a program.

Fig. 1 illustrates the time-dependent dynamics of concentrations for four substances during the methanogenesis process. Each line in the graph meets the changes in concentrations of one of the substances: 1. Blue graph: hydrogen concentration S_H decreases over time. It seems expectable since hydrogen is actively involved in the biochemical reactions of methanogenesis and consumed

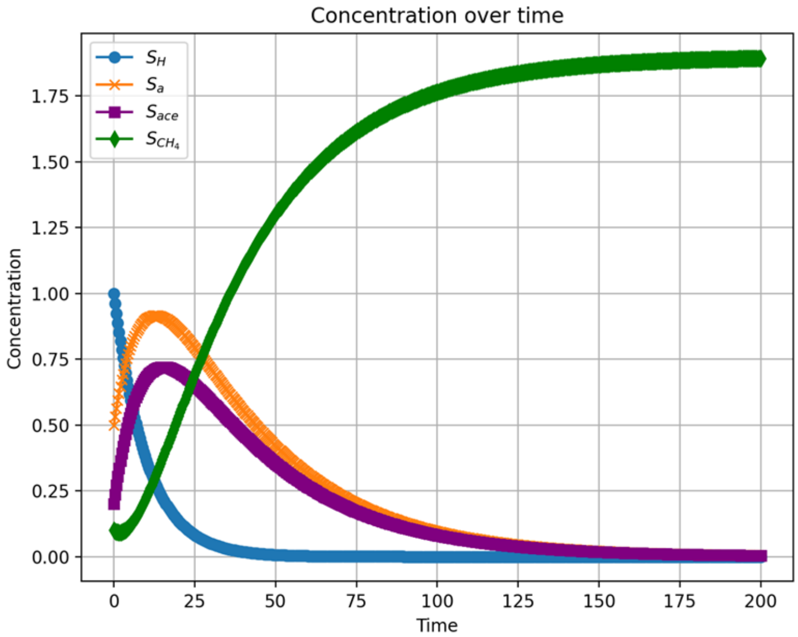


Fig. 1: Experimental results of concentrations over time.

during the methanogenesis process. 2. Orange graph: the concentration of the intermediate S_a initially increases, reaching a peak. Then it sees a considerable decrease. The process indicates that, at first the intermediate substance is formed from hydrogen, and it is then used in subsequent reactions. 3. Purple graph: acetate concentration S_{ace} at first also increases, reaching its peak, and then experiences a diminish. Like the intermediate substance, acetate is formed and used during the methanogenesis process. 4. Green graph: methane concentration S_{CH_4} increases, reaching the plateau. Then the process culminated in methane accumulation, which remains as the final product that is not used in the subsequent reactions.

The process can be described on the graph as follows: hydrogen S_H is actively used at the early stages, as it is readily seen from its exponential decrease; intermediate substances S_a and acetate S_{ace} are initially formed from hydrogen, and reach the maximum concentration, then begin to decrease as they are further used; methane S_{CH_4} is accumulated as the reaction proceeds and its concentration grows monotonously, reaching the saturation state. Fig. 2 visually illustrates the kinetics of chemical reactions in methanogenesis, highlighting the time-dependent changes in the concentration of different substances.[27]

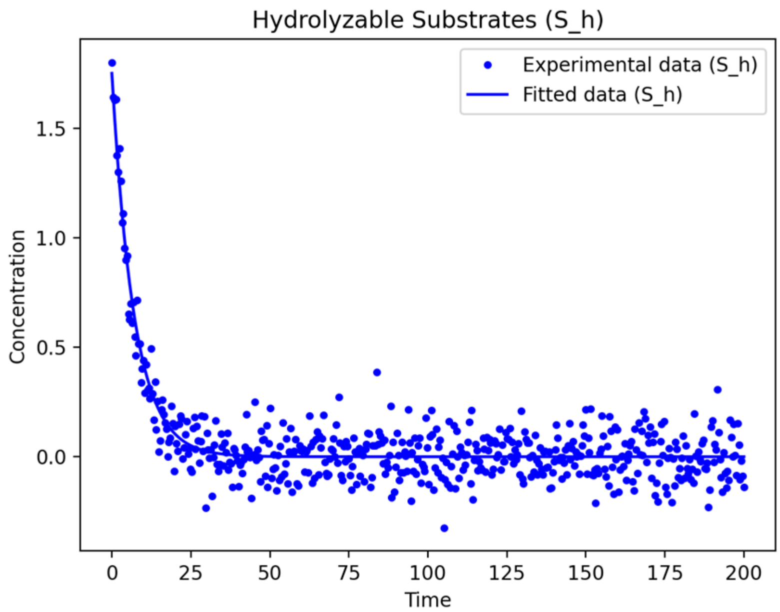


Fig. 2: Experimental results of hydrolyzable substrates.

Fig. 2 illustrates the time-dependent dynamics of concentrations of hydrolyzable substrates (S_h). The detailed description of the graph is as follows: title: the graph title is "Hydrolyzable Substrates (S_h)"; X-axis: The X-axis is denoted as "Time" and indicates the time measured in some units, ranging from 0 to 200; Y-axis: The Y-axis is denoted as "Concentration" and measures the concentrations of hydrolyzable substrates, varied from 0 to approximately 1.6; dot plot: The graph contains blue dots, presenting the experimental data of hydrolyzable substrates (S_h) at different time intervals; approximate data: The blue line represents approximate data of concentrations of hydrolyzable substrates (S_h). The line aligns with the trend observed in the experimental measurements; legend: The legend on the graph indicates that blue dots align with "Experimental data (S_h)" (experimental data), and blue lines align with "Fitted data (S_h)" (approximate data). According to Fig. 3, the concentration of hydrolyzable substrate declines rapidly at first, and then it levels off, maintaining relatively constant low concentrations over time.

Fig. 3 illustrates the time-dependent dynamics of concentrations of volatile fatty acids (S_a) over the time. Below is a detailed description of the graph: Title: The graph is named "Volatile Fatty Acids (S_a)"; X-axis: The X-axis is denoted as "Time" and indicates the time measured in some units, ranging from 0 to 200; Y axis: The Y-axis is denoted as "Concentration" and measures the concentrations of volatile fatty acids, varied from -0.2 to approximate 0.8; dot plot: The graph contains red dots, presenting the experimental data of volatile fatty acids (S_a) at different time intervals; approximate data: Approximate data of volatile fatty acids (S_a) is represented bya red line which follows the pattern seen in experimental dots; legend: The legend on the graph indicates that red dots align with "Experimental data (S_h)" (experimental data), and red lines align with "Fitted data (S_h)" (approximate data). In Fig. 4, the concentration of volatile fatty acids increases rapidly at first before reaching its highest point at around 20. Despite the subsequent decline, the line levels off, maintaining relatively constant low concentrations over time.[28]

Fig. 4 represents the time-dependent dynamics of acetate concentration (S_ace). A detailed explanation is as follows: Title: The graph is named "Acetate (S_ace)"; X-axis: The X-axis is denoted as "Time" and indicates the time measured in some units, ranging from 0 to 200; Y-axis: The Y-axis is denoted as "Concentration" and measures the acetate concentrations, varied from -0.2 to approximate 1.0; dot plot. The graph contains green dots, presenting the experimental data of acetate concentration (S_ace) at different time intervals; approximate data: Approximate data of acetate (S_ace) is represented by a green line which follows the pattern seen in experimental dots; legend: The legend on the graph indicates that green dots align with "Experimental data (S_ace)" (experimental data), and green lines align with "Fitted data (S_ace)" (approximate data). In Fig. 5, the acetate concentration increases rapidly at first before reaching its highest point at around 25. Despite the subsequent decline, the line levels off, maintaining relatively constant low

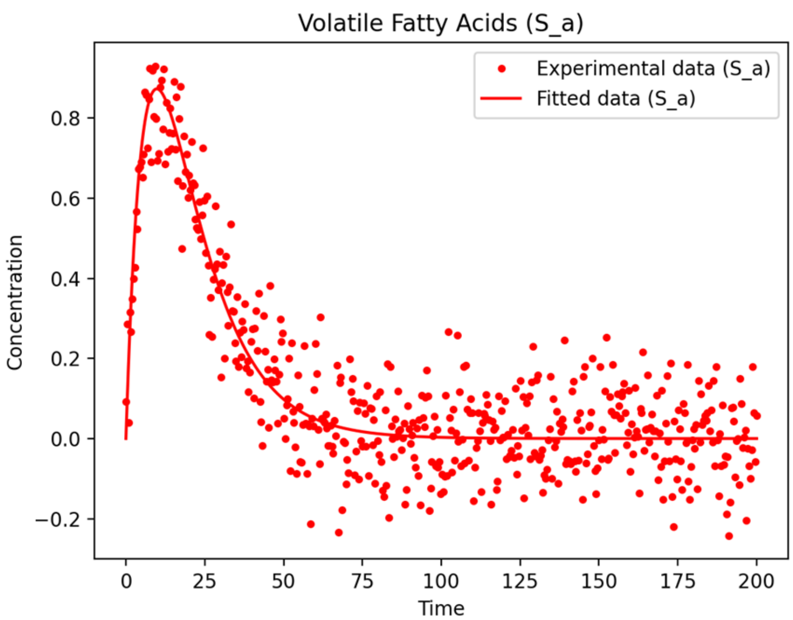


Fig. 3: Experimental data of volatile fatty acids concentration.

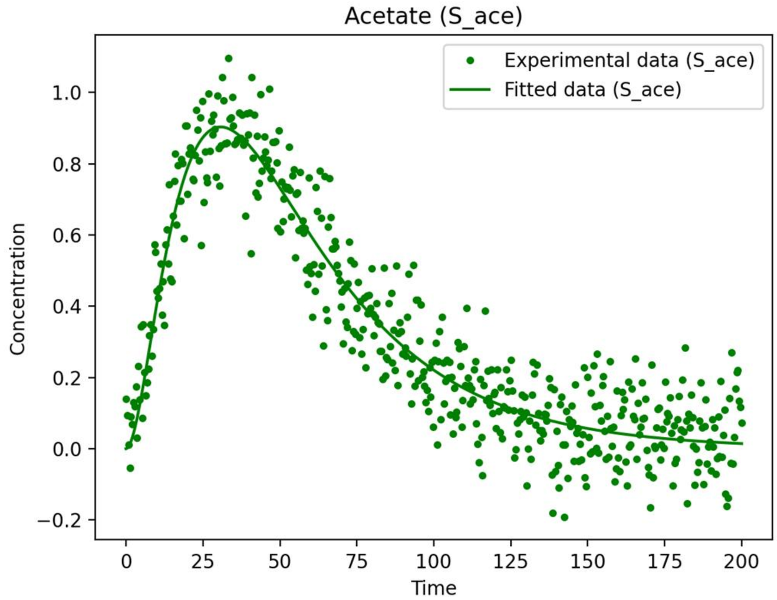


Fig. 4: Experimental data of acetate concentration.

concentrations over time.[29] The acetate level increases sharply to its maximum value, after which, despite a slight decrease, it remains relatively stable over time. The acetate concentration quickly reaches a peak value, and then, despite a slight drop, remains relatively stable over time.

Fig. 5 represents the time-dependent dynamics of methane concentration (S_CH4). A detailed explanation of the graph is as follows: title: The graph is named as "Methane (S_CH4)"; X-axis: The X-axis is denoted as "Time" and indicates the time measured in some units, ranging from 0 to 200; Y-axis: The Y-axis is denoted as "Concentration" and measures the methane concentrations, varied from 0 to approximate 2.0; dot plot. The graph contains black dots, presenting the experimental data of methane concentration (S_ace) at different time intervals; approximate data: Approximate data of methane (S_CH4) is represented by a black line which follows the pattern seen in experimental dots; legend: The legend on the graph indicates that black dots align with "Experimental data (S_CH4)" (experimental data), and black lines align with "Fitted data (S_CH4)" (approximate data). Fig. 5 illustrates a gradual increase in methane concentration over time, starting from 0 and reaching approximately 2.0 by the end of the observed period.[30]

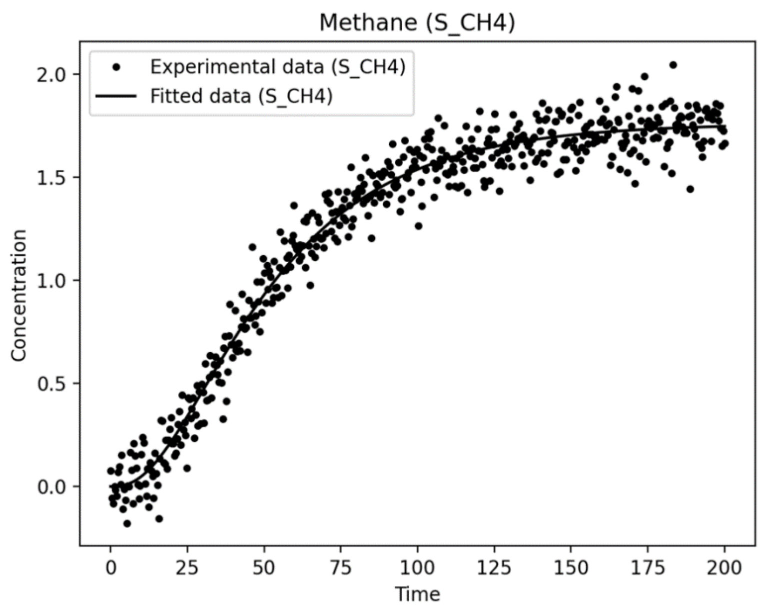


Fig. 5: Experimental data of methane concentration.

The description of Fig. 6 "Hydrolyzable Substrates (S_h)" Fig. 6a illustrates the time-dependent dynamics of hydrolyzable substrates S_h, representing both theoretical and experimental results. The graph demonstrates three distinct datasets. The theoretical model that depicts the change in concentration of hydrolyzable substrate S_h over time. The theoretical curve illustrates an exponential decrease in concentration, starting with a high initial concentration, and decreasing to almost zero values. The experimental data, obtained during actual measurement. The dots illustrate actual observations on the concentration of hydrolyzable substrates S_h at various time intervals. The experimental data shows a significant deviation around the theoretical curve which indicates the variability of measurements or effects of external factors. The Fitted data adjusted data are the result of applying the model to the experimental data, aiming to minimize deviations, it indicates the model's consistency with experimental data, considering the variability among experimental dots.

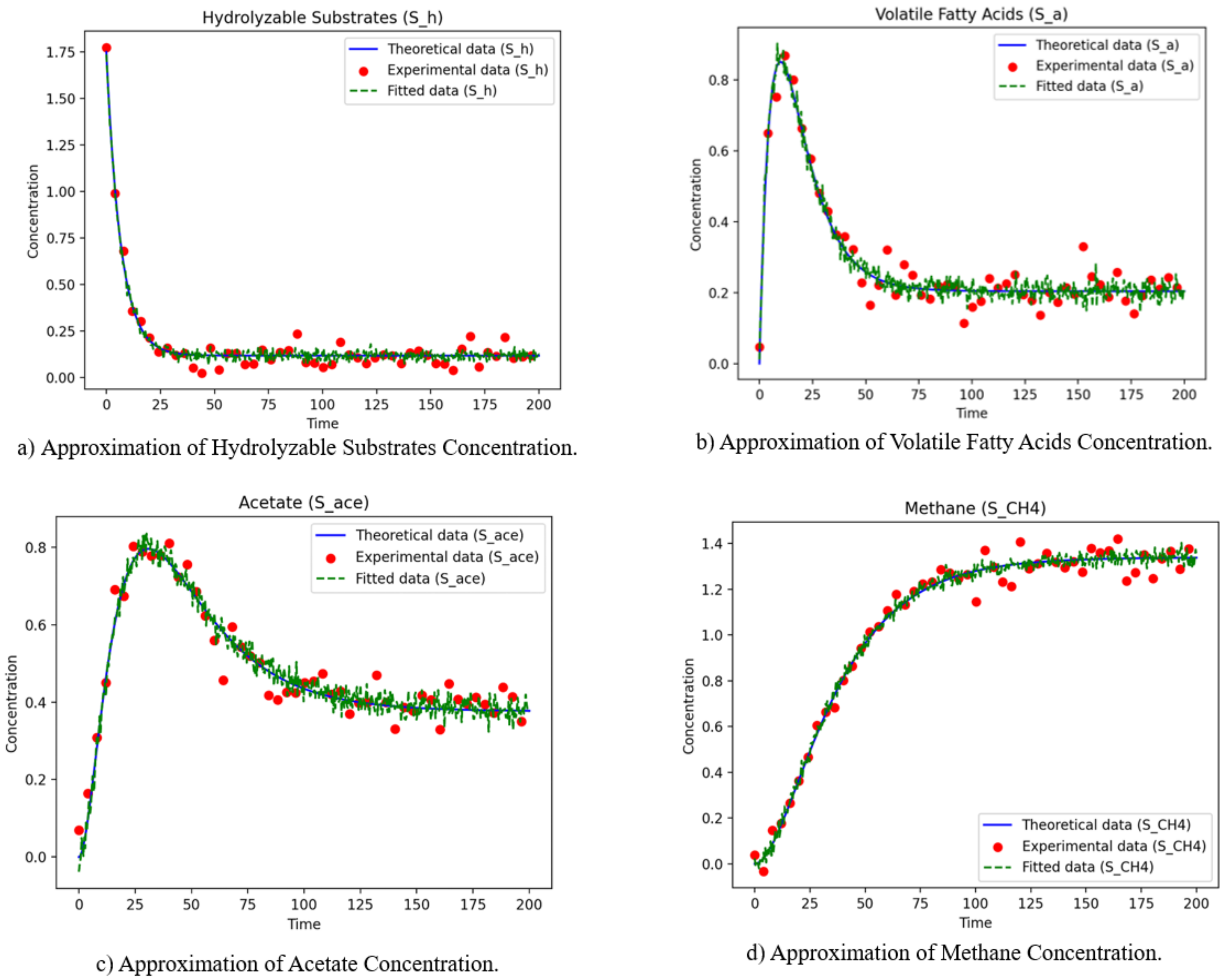
Analysis of Fig. 6a: initial concentration: Initially in the process (time = 0) concentration of hydrolyzable substrates is high (around 1.75 units); period of sharp decline: In the first 25 time units, there is a notable decline in concentration, as evidenced by both theoretical and experimental findings; steady condition: after 50 time units, the concentration stabilizes and remains at the lowest level (around 0.25 units) till the end of the observed period.

According to the Fig 6a, the theoretical model accurately represents the overall pattern of declining hydrolyzable substrate concentrations. The experimental findings generally align with the theoretical curve despite some deviations. Adjusting the model to fit experimental data improves compliance and provides a more precise understanding of hydrolysis substrates. This analysis is important for enhancing the models and improving the accuracy of prediction in actual conditions.

Fig. 6b demonstrates the changes in concentration of volatile fatty acids S_a over time, including both theoretical and experimental findings. Three distinct datasets can be seen in the graph. The theoretical model that depicts, the change in concentration of volatile fatty acids S_a over time. The theoretical curve illustrates an exponential increase in concentration, reaching the peak, and then decreasing and stabilizing.The experimental data, obtained during actual measurement. The dots illustrate actual observations on the concentration of volatile fatty acids S_a at various time intervals. The experimental data shows a slight deviation around the theoretical curve.

The Fitted data adjusted data are the result of applying the model to the experimental data, aiming to minimize deviations. This indicates the model's consistency with experimental data, considering the dot dispersion. Analysis of the graph in Fig. 6b: initial concentration: At the start of the process (time = 0), the concentration of volatile fatty acids is almost zero; concentration growth: In the first 25 time units, there is a notable decline in concentration, reaching the maximum of 0.8 units; reduction phase: After reaching the maximum, it starts to decline; stable condition: After 75 time units, concentration steadies at about 0.2 units and maintains the level till the end of observation. Fig. 6b demonstrates that the theoretical model accurately represents the overall dynamics of changes in the concentration of volatile fatty acids. The experimental findings generally align with the theoretical curve despite some deviations. Adjusting the model to fit experimental data improves compliance and provides a more precise understanding of the concentration change process. This analysis is important for enhancing the models and improving the accuracy of prediction in actual conditions. It can facilitate the enhancement of biogas plant operations.[29]

Fig. 6c depicts the time–based dynamics of acetate concentration, S_{ace} including both theoretical and experimental results. Three distinct datasets can be seen in the graph. This is a theoretical model that depicts the change in acetate concentration S_{ace} over time. The theoretical curve illustrates an exponential increase in concentration, reaching the peak, then decreasing and stabilizing. These are experimental results, recorded during the measurements. The dots present the actual observations on the concentration of acetate S_{ace} at various time intervals. The experimental data shows a slight deviation around the theoretical curve. These adjusted data are the result of applying the model to the experimental data, aiming to minimize deviations. This indicates the model's consistency with experimental data, considering the dot dispersion. Analysis of Fig. 6c: initial concentration: Initially in the process (time = 0) concentration of acetate is around zero; concentration growth: In the first 50 time units, there is considerable growth in the concentration, reaching the peak of 0.8 units; reduction phase: As soon as concentration reaches the peak, it begins to fall; steady state: after 100-time units the concentration reaches the level of 0.4 units and remains stable till the end of the observed period. In Fig. 6c, the theoretical model accurately represents the overall pattern of acetate concentrations. The experimental findings generally align with the theoretical curve despite some deviations. Adjusting the model to fit experimental data improves compliance and provides a more precise understanding of changes in concentration. The analysis is important for enhancing the models and improving the



a) Approximation of Hydrolyzable Substrates Concentration.

b) Approximation of Volatile Fatty Acids Concentration.

c) Approximation of Acetate Concentration.

d) Approximation of Methane Concentration.

Fig. 6: Dynamics of concentrations of key components involved in biochemical stages of methanogenesis. (a) Hydrolyzable substrates, (b) Volatile fatty acids, (c) Acetate, and (d) Methane.

accuracy of prediction in actual conditions. This can facilitate to optimization of the processes in biogas plants.[31]

Fig. 6d depicts the time–based dynamics of methane concentration S_{CH_4} including both theoretical and experimental results. Three distinct datasets can be seen in the graph. This is a theoretical model that depicts the change in methane concentration S_{CH_4} The theoretical curve demonstrates that methane concentration gradually increases, reaching the plateau. These are actual measured data, collected during the experiment. The dots present the methane concentration S_{CH_4} at various time intervals. The experimental data shows a slight deviation around the theoretical curve. This is data obtained by fitting the model to experimental data to minimize deviations. This indicates the model's consistency with experimental data, considering the dispersion of the observed dots.[29] Analysis of the graph in Fig. 6d: Initial concentration: Initially in the process (time = 0) concentration of methane is around zero.concentration level growth: In the first 50 time units, there is considerable growth in the concentration, reaching the peak of 0.8 units; saturation period: after 50-time units, the methane concentration continuously increases despite some retardation; stationary condition: after 125 time units, the concentration is set at about 1.3 units and remains constant until the end of the monitoring timeframe.

In Fig. 6d, the theoretical model accurately represents the overall pattern of acetate concentrations. The experimental findings generally align with the theoretical curve despite some deviations. Adjusting the model to fit experimental data improves compliance and provides a more precise understanding of changes in concentration. The analysis is important for enhancing the models and improving the accuracy of prediction in actual conditions. This can facilitate to optimization of the processes in biogas plants.[31] Fig. 6 depicts the concentration of substrates, volatile fatty acids, acetates, and methane over time with three separate datasets: theoretical data, experimental data, and approximate data. A detailed explanation of the process after conducting mathematical and numerical calculations is depicted on the graph:

Title and axis title: substrates, volatile fatty acids, acetate, and methane; X-axis: time; Y axis: Concentration.

(1) Description of the data

– theoretical data: A solid blue line presents this data. This shows the expected concentration of hydrolyzable substrates in time-based on a theoretical model.

– experimental data: this data is presented with red dots. The dots are the actual measurements of hydrolyzable substrates, obtained during the experiment.

– aapproximate data: This data is illustrated with a green dotted line. This demonstrates the concentration of hydrolyzable substrates, obtained through approximate models to experimental data.

(2) Observation

– initially (unit = 0) concentration of hydrolyzable substrates is high;

– there is a rapid change in concentration at the initial period;

– once the initial shift occurs, concentration stabilizes, and fluctuates between high and low values, respectively, for the rest of the observation period.

(3) Approximation of the model

The approximated values closely match the experimental data showing that the model used for approximation accurately reflects the observed behavior.

The approximate lines demonstrate the results of the approximation of experimental data using artificial methods including machine learning and neural networks. The effectiveness of approximation in green dotted lines derived from Fig. 6 also aligns well with experimental data. This proves that artificial intelligence methods succeed in tackling approximation issues. In terms of theoretical data, it also follows the overall trend of experimental data.

Fig. 6 effectively compares the theoretical predictions, experimental observations, and results of the approximation model for the concentration of hydrolyzable substrates over time. Strong agreement between the approximated data and the experimental data confirms that the model used for approximation, as theoretical data can offer a solid approximation of the system dynamics. Fig. 6 illustrates the efficiency of implementing artificial intelligence methods for approximation and predicting thermal processes in biogas planting which is an essential step in optimizing their functions.

4. Discussion

The research addressed two key issues, including mathematical modeling of biogas plants, integrating artificial intelligence (AI), and monitoring and enhancing the performance of biogas plants. The first research question was about the mathematical modeling of biogas plants. Mathematical modeling in biogas planting is important for predicting thermal regimes and enhancing system functionality. Biogas planting is a challenging process where multiple variables, including temperature, moisture, raw material composition, and parameters of microbiological processes, influence output results. The model should consider all these factors for precise prediction and process management.[32]

The main elements of mathematical models are as follows: Thermal balance: It includes equations for describing thermal transfer within the system. The equations account for the heat generated when organic material decomposes, and the heat released into the environment. Kinetics of biochemical reactions: The model should consider the speed at which organic material breaks down and biogas production. It includes microbiological processes that occur during different stages of anaerobic decay. Mass transfer processes: These include the transfer of gas (methane, carbon dioxide, and others), and the flow of liquid and solid components within the reactor. Hydrodynamics: It accounts for the movement of liquid and gas within the reactor, which is crucial for the consistent distribution of temperature and nutrients. Control parameters: These include controllable variables, namely the speed of raw materials, the temperature within the reactor, and mixing conditions. These models facilitate the prediction of biogas output and assess the efficiency of planting under different conditions. Complex mathematical equations are used to describe the system will be addressed with numerical methods, such as the finite element method (FEM) and the Monte Carlo method, to obtain accurate and reliable results.

The second research question was aimed at applying artificial intelligence to biogas plant control. Implementing AI not only provides predictions but also optimizes the process of biomass recycling, which results in a more stable and effective biogas plant process.[29] Thermal regime forecasting and optimization: Machine learning, and neural networks can be used for analyzing big data obtained from sensors and predicting changes in thermal regimes. It assists in timely adjusting installation parameters to maintain optimal conditions.

We performed a quantitative comparison between the model's predictions and experimental results. As shown in Table 2, the model achieved high predictive accuracy across key indicators, including methane and acetate concentrations, temperature, and biogas output. The R^2 values ranged from 0.96 to 0.99, confirming strong alignment with real-world measurements. The relative error remained under 6% for all variables, highlighting the model's robustness and practical applicability under actual plant conditions. Process

Table 2: Quantitative comparison between model predictions and experimental data under real operating conditions.

Indicator	Absolute error	Relative error (%)	R^2 value
Methane concentration (S^{CH_4}) [mol/L]	0.04	3.05	0.985
Acetate concentration (S^{ace}) [mol/L]	0.02	2.5	0.972
Volatile fatty acids (S^a) [mol/L]	0.04	5.71	0.96
Reactor temperature (T) [°C]	0.4	1.09	0.989
Biogas output [m³/day]	3	2.46	0.979

management automation: AI can autonomously control the various aspects of biogas plant processes, such as feedstock, temperature and moisture control, and mixing speed. It reduces the necessity of human intervention and increases the system's reliability. Failure identification and prediction: AI algorithms can analyze equipment operation patterns and predicting failures before their occurrence. This allows for preventative maintenance and reduces the risk of accidents.

Despite the obtained results, the current model has several limitations. First, the mathematical and AI components were trained and validated using data from a limited number of biogas plant configurations, which may restrict generalizability to other systems with different operational scales or feedstocks. Second, some physicochemical assumptions, such as constant heat transfer coefficients and simplified microbial, kinetics may not fully capture real-world complexity. Additionally, the accuracy of the AI models depends on the quality and diversity of input data; therefore, prediction errors may increase in unobserved operating ranges.

5. Conclusions

During the research, a mathematical model for predicting the thermal behaviors and functionality of a biogas plant was created and studied. It has made considerable progress in understanding the process occurring in such planting. The main findings of the research could confirm the model's efficiency in predicting thermal characteristics and optimizing the installation activities in various operating conditions. Moreover, it was found that the influence of key parameters including raw material composition, technical parameters, and external conditions on the biogas plant's performance was revealed. The result is an important step towards enhancing sustainability and the efficiency of biogas production processes which lead to operational cost reduction and improvement in ecological indicators.[30]

Implementing mathematical models offers a potential for further research and development in the renewable energy field. Developing precise predictive and process management methods in biogas plants facilitates the creation of sustainable and competitive technologies based on using renewable resources. Throughout the study, by using AI methods, a mathematical model was designed to predict the thermal regime and optimize the function of biogas plants. The primary findings and outcomes of the study encompass the following aspects. A complex mathematical model was developed that described the thermal process within the biogas plant. The model considered the main physical and chemical parameters, including heat transmission, reaction kinetics, and dynamics in temperature change.

AI methods including neural networks and machine learning algorithms were employed to improve the precise predictive analysis and biogas plant optimization. The methods helped to significantly improve the accuracy of approximation in experimental data and adapt the model to the actual operating conditions. The adoption of a hybrid model that fuses traditional mathematical methods with AI approaches demonstrated high efficiency in solving prediction issues and thermal regime optimization. This facilitated more accurate and reliable outcomes, which is particularly significant for real-world applications.

The developed ‘model and algorithms were tested using actual data, which confirmed its viability in practical settings. Utilizing these methods in the management of biogas plants assists to improve their efficiency, reduce operational costs, and increase energy output.[31] Future improvements will focus on expanding the dataset to include a wider variety of biogas plants, integrating real-time sensor data using IoT frameworks, and refining the model to include dynamic microbial community responses. Incorporating uncertainty quantification and robust sensitivity analysis will also strengthen the model's reliability for industrial applications.

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Conflict of interest

There are no conflicts to declare.

Supporting information

Not applicable.

CRediT Statement

Omirlan Auelbekov: Conceptualization, Methodology, Formal analysis, Resources, Writing supervision, Writing - reviewing and editing. Ainur Kozbakova: Conceptualization, Methodology, Formal analysis, Writing supervision, Funding acquisition. Writing - review & editing. Kairat Yesentaev: Formal analysis, Software, Data curation, Data visualization, Writing - reviewing and editing: participated in the preparation of the technical sections of the article. Timur Merembayev: Methodology, Software, Data curation, Writing - reviewing and editing: participated in the preparation of the technical sections of the article. Kuanyshbek Igibaev: Formal analysis, Software, Data curation, Data visualization.

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