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Enhancing Sustainable Biogas Generation Through a Real-Time Digital Twin of a Modular Bioreactor

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Abstract

This article presents the design and research of a modular horizontal tubular bioreactor for efficient biogas production based on anaerobic digestion technology. The study combines a digital twin implemented in the MATLAB/Simulink environment with a physical bioreactor equipped with a sensor and control system. The developed mathematical model describes the biochemical processes of acidogenesis and methanogenesis, the thermal regime and the sensitivity of the system to key parameters. Numerical modeling and visualization methods were used for the analysis. The experiments were carried out for 30 days at a mesophilic temperature of 37 ° C, repeated three times to increase reliability. The raw material used was a mixture of cattle manure and food waste in a 3:1 ratio, with a total volume of 60 liters. Readings from temperature, pH, and methane sensors were taken every 10 minutes. Experimental data confirmed the high efficiency of the design: removal of up to 70.5% of volatile substances and methane yield of up to 80.5%. Predictive analysis has shown that the digital twin is able to predict the behavior of the system and apply corrective actions in real time. The novelty of the work lies in the integration of a digital twin with a physical bioreactor in real time through industrial communication protocols.

Keywords: Biogas, Anaerobic Digestion, Bioreactor, Biomass, Mathematical Model, MATLAB, Simulink, Renewable Energy

1. Introduction

Biogas can be utilized as fuel for heat and electricity generation. Alternatively, biogas can be upgraded and injected into the gas grid (biomethane). By 2030, biogas and biomethane are gaining increasing distribution as renewable energy sources. The price and availability of biomass are primary uncertainties. For biomass, the gas industry must compete with the food and electricity industries; and further increases in demand could lead to price increases. Recently, the demand for Anaerobic Digestion (AD) biogas technology has been gradually increasing due to its energy and environmental benefits.

One of the major environmental challenges facing today's society is the continuous increase in the generation of solid organic waste and wastewater, and their disposal. In many countries, sustainable waste management, as well as waste prevention and reduction, have become necessary political priorities, representing a significant element of joint efforts to reduce pollution and mitigate the effects of global climate change [1], [2]. Intelligent management of organic waste allows for energy recovery, regardless of whether it is carried out by traditional incineration or through landfilling and anaerobic digestion [3], [4]. Thus, a candidate for energy recovery from organic waste is biogas recovery, whether it is generated in landfills or during anaerobic digestion [5]. The anaerobic digestion process, implemented in anaerobic biorefineries, can play a significant role in addressing fundamental challenges of our society: waste and wastewater management, their treatment, and the production of renewable energy.

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The biodigester appears to be a candidate for a clean development mechanism, required by the United Nations, and contributes to the reduction of pollutant emissions into the atmosphere [6]. Furthermore, it contributes to sustainable development at the local level by processing organic waste generated as a result of established activities, which allows not only to produce energy but also to use waste as biofertilizers, reduces electricity generation from non-renewable sources, and reduces water use in technological processes [7], [8], [9], [10]. Anaerobic digestion appears to be one of the solutions to these problems, as well as an attempt at the secondary use of Municipal Solid Waste (MSW). It is well known that anaerobic digestion is a process in which organic waste is biologically transformed by a microbial consortium in the absence of oxygen [11]. In addition to stabilizing the organic load of waste, this process produces products such as biogas, rich in methane, which can be used as a soil conditioner, historically used for sludge stabilization in wastewater treatment, although this is not the only viable use for processing any substances [12].

Besides the potential for renewable energy production, anaerobic digestion is becoming increasingly researched and known due to several factors, such as the limitation of landfill volumes and the energy supply of small settlements far from urban centers. Another undeniable advantage is the minimal formation of sludge. In anaerobic digestion, about 10% of the organic residue is converted into sludge, and the remaining 90% is used as biogas. It is also essential to emphasize the use of anaerobic processes on both small and large scales with low implementation costs, low area requirements, and good stability to high organic loads [13]. Consequently, biogas production and the development of biomethane production technologies are encouraged by many countries as an alternative to electricity generation or cogeneration in internal combustion engines [14], [15], [16], [17].

This paper [18] explores the potential resources for biogas production in the Republic of Kazakhstan. It provides annual energy estimates of biogas derived from livestock manure across various regions of the country. Furthermore, it includes calculations of biogas generation from municipal solid waste and sewage sludge within Kazakhstan. The paper [19] presents a simplified one-stage mathematical model of anaerobic digestion kinetics, built on mass balance equations. Simulation studies were carried out using initial data. The simulation results obtained using Simulink were used to calibrate the maximum growth rate of microorganisms in order to optimally match the model data with experimental results. The paper [20] provides examples and computer code for MATLAB/Simulink, and also discusses aspects related to ordinary differential equations and differential-algebraic equations. Implementations related to system stiffness and changing time constants, mass balance, acid-base equilibrium, as well as algebraic solutions for pH and other problematic state variables are considered. Numerical solutions and analysis of simulation time are carried out. The main conclusion is that with proper implementation, the advanced ADM1 provides high-quality simulation, which also contributes to the dynamic modeling of the entire process, including noise, discrete subsystems, and other aspects, without significant limitations related to computational costs.

The paper [21] examines the main challenges in applying anaerobic digestion in whole-plant modeling, which requires improving characteristics, increasing the efficiency of new technologies, and considering the key role of interconnected phosphorus-sulfur-iron processes throughout the cycle. The review concludes that anaerobic modeling is becoming increasingly complex and places growing demands on model developers. However, the basic principles of biochemical and physicochemical processes, metabolism conservation, and mechanistic understanding remain important for solving new problems. In the study [22], a modeling tool based on the Anaerobic Digestion Model No. 1 (ADM1) was developed, capable of simulating the Thermodynamic System (TS) and the mass/volume dynamics of the reactor in the HS-AD OFMSW process. Four hypotheses were used for modeling, including the effect of apparent concentrations at high TS values. The model successfully simulated the operation of HS-AD OFMSW in batch and continuous modes, including changes in TS, reactor mass, ammonia level, and volatile fatty acid concentrations.

The paper [23] outlines the principle of operation of a biogas energy system, as well as the design and detailed mathematical modeling of each of its segments. Additionally, an adaptive control mechanism was implemented to improve system stability. The MATLAB/Simulink environment was used as a platform for the development of the entire biogas-powered energy system, which made it possible to obtain various operating parameters of the system. The paper [24] considers the principles of operation of a biogas energy system, as well as its design and mathematical modeling of each segment. In the process, an adaptive control mechanism was developed and implemented to improve system stability. The MATLAB/Simulink environment was used to create the model, which allowed for detailed calculations and analysis of various system parameters.

The study [25] conducted a techno-economic analysis of a hybrid microgrid system that runs on diesel fuel and biogas. The microgrid system was modeled using MATLAB/SIMULINK, and HOMER software was used for system optimization. Also, within the framework of the work, AD processes were developed and modeled using Simulink to estimate the methane yield from the reactor. In the paper [26], time series-based modeling is developed and investigated, which provides a deep understanding of technological fluctuations in the anaerobic digestion process. A dynamic model based on a modified Hill model using MATLAB was also created, designed to predict biomethane production using time series. This model allows predicting biomethane production in both batch and continuous processes, on different substrates and under various conditions, such as total solids content, loading rate, and operating time. Using the proposed model, it is possible to determine a stable and optimal loading rate that ensures methane production at minimal cost.

The study [27] presents a new mathematical model for mesophilic anaerobic co-digestion in batch reactors. The uniqueness of the model lies in its ability to combine completeness and simplicity, implemented in the MATLAB environment, which ensures accuracy and user-friendliness. Special attention is paid to crucial factors such as total VFA and methane formation, which distinguishes the model in the field of anaerobic digestion. The practical applicability and accuracy of the model make it a valuable tool for optimizing real-world waste management and renewable energy production processes, which can contribute to increased methane yield and overall biogas production. This study aims to develop, model, and experimentally validate an intelligent control system for a modular bioreactor based on a digital twin, providing monitoring, prediction, and optimization of anaerobic digestion processes for efficient biogas production in conditions of limited access to centralized energy sources.

2. Research Methodology Mathematical Model

A simplified model of the anaerobic process is considered, in which the organic substrate S1 (in gCOD/L) degrades into intermediate products (S2, in mmoleVFA/L) with the help of acidogenic bacteria (X1, in gCOD/L). Further, S2 is decomposed into methane (CH4, in L/d) by methanogenic microorganisms (X2, in gCOD/L). This kinetic model describes the biological reactions [28]:

$$k_1 S_1 \overset{r_1}{\rightarrow} X_1 + k_2 S_2 \text{ (acidogenesis)} \tag{1}$$

$$\mathrm{k_3 S_2 \overset{r_2}{\rightarrow} X_2 + k_4 CH_4} \text{ (methanogenesis)} \tag{2}$$

k1 (gCODS1 / gCODX1), k2 (mmoleVFA/gCODX1), k3 (mmoleVFA/gCODX2) and k4 (mmoleCH4 /gCODX2) - the stoichiometric coefficients of the reactions. The growth rates of bacteria are related to the biological processes [28]:

$$\mathrm{r1(r1 = \mu X1)} \text{ и } \mathrm{r2\ (r2 = \mu X2)} \tag{3}$$

μ1 и μ2 (d-1) - the growth rates of acidogenesis and methanogenesis, respectively. The system of differential equations describing the mass balance in a continuous process has the following form [29]:

$$\frac{dX_1}{dt} = X_1(\mu_1 - D) \text{ (acidogenic biomass)} \tag{4}$$

$$\frac{dX_2}{dt} = X_2(\mu_2 - D) \text{ (methanogenic biomass)} \tag{5}$$

$$\frac{dS_1}{dt} = D(S_1^{in} - S_1) - k_1\mu_1 X_1 \text{ (organic substrate)} \tag{6}$$

$$\frac{dS_2}{dt} = D(S_2^{in} - S_2) - k_2\mu_1 X_1 - k_3\mu_2 X_2 \text{ (fatty acids)} \tag{7}$$

D (D = Q/V; в d-1) - the dilution rate defined by the ratio between the influent flow rate Q and the reactor volume V V, S_1^{in}и S_2^{in} - the influent concentrations of organic substrate and fatty acids, respectively. In addition to the structural diagrams shown in Figures 3, 5, and 7, this section provides functional simulation results illustrating the operation of the control system in the event of disturbances and changes in the setpoint. The model was tested in MATLAB/Simulink for a duration of 3600 seconds, corresponding to one hour of simulated time. During the simulation, the setpoint temperature was maintained at 37 °C. At time t = 1200 seconds, a short-term disturbance was introduced by decreasing the ambient temperature by 4 °C. To regulate the system and respond to this disturbance, a PID controller was implemented with the following coefficients: KP = 2.5, KI = 0.3, and KD = 0.1.

Under normal conditions, without disturbances, the controller demonstrates stable behavior and reaches the setpoint in less than 300 seconds. The maximum overshoot is no more than 0.7 °C, and the steady—state deviation is less than 0.2 °C, which meets the requirements of stable operation of the bioreactor. When the external temperature decreases by 4 °C at time t = 1200 s, a short-term decrease in the internal temperature of the reactor by 0.8 °C is observed. The system restores the preset level in less than 200 seconds, thanks to the corrective action of the PID controller. The temperature graph shows a rapid suppression of deviation without fluctuations and residual drift. When the regulator is switched off (the model is in an open loop), the decrease in reactor temperature with a similar disturbance is more than 3.2 °C and is not compensated for during the entire simulation interval. The presented functional results confirm the ability of the proposed controller to effectively monitor the setpoint and respond to disturbances, ensuring stability, accuracy and adaptability of the thermal regime of the bioreactor. The kinetics of acidogenic bacteria are described by the Monod equation [30]:

$$\mu_1 = \mu_{1max} \frac{S_1}{K_{S_1} + S_1} \text{ (kinetics of acidogenic bacteria)} \tag{8}$$

For methanogenic bacteria, Haldane kinetics are used, considering inhibition [31]:

$$\mu_2 = \mu_{2max} \frac{S_1}{K_{S_2} + S_2 + S_2^2/K_I} \text{ (kinetics of methanogenic bacteria)} \tag{9}$$

μ_{1max} и μ_{2max} – the maximum growth rates of bacteria, and K_{S_1}, K_{S_2} и K_I - the half-saturation and inhibition constants for organic matter and fatty acids. In the presented work, the Haldane kinetic model is used in equation (9) to describe the inhibition of the growth of methanogenic microorganisms at an increased concentration of intermediates. However, the article does not specify the numerical values of key parameters such as the KIK_IKI inhibition coefficient, the maximum growth rate and the semi-saturated concentration. The lack of these data makes it impossible to reproduce the model, verify the strength of the claimed inhibitory effect, and compare the results with similar data presented in other empirical studies. To increase the scientific reproducibility of the model in future versions, it is recommended to include a table with numerical values of all parameters and ranges of their variation in sensitive analysis. Methane is a poorly soluble gas, so all CH4 produced is released as biogas. The methane yield is described by the equation [32]:

$$q_M = k_4 \mu_2 X_2 \quad \text{(methane production)} \tag{10}$$

For sensitivity analysis of the process to parameter changes, a dimensionless sensitivity is introduced, defined by the equation [33]:

$$\sigma_q = \frac{1}{t_f} \int \frac{z_q + \Delta_q - z_q}{z_q} dt \qquad \text{(sensitivity analysis of methane production)} \tag{11}$$

zq – the investigated variable, Δ_q – the change in the parameter, t_f- the final time.

The equation describes the thermal balance of a reactor, taking into account three factors: internal heat generation, heat loss through insulation, and heat exchange between phases during mixing. The left part reflects the rate of temperature change, and the right part is the sum of all heat fluxes affecting the system. This makes it possible to accurately simulate temperature dynamics in real time.

$$mC_p \frac{dT(t)}{dt} = Q_{gen}(t) - \frac{T(t) - T_{env}(t)}{R_{insul}(t)} + h_{mix} A [T_{fluid}(t) T_{solid}(t)]_{int} \tag{12}$$

This model allows predicting methane yield and the dynamics of the bioreactor operation, as well as identifying key factors affecting process efficiency. The main simulation results are summarized in table 1.

Table 1. Kinetic and Stoichiometric Parameters Used in the Model

Parameter	Description	Value (unit)
k1	Stoichiometric coefficient of substrate conversion to acidogenic biomass	0.75 (gCOD/gCOD)
k2	Stoichiometric coefficient of substrate conversion to VFAs	1.20 (mmolVFA/gCOD)
k3	Stoichiometric coefficient of VFA conversion to methanogenic biomass	0.95 (mmolVFA/gCOD)
k4	Stoichiometric coefficient of methane formation	0.30 (mmolCH4/gCOD)
μ1	Maximum growth rate of acidogenic bacteria	0.60 (1/day)
μ2	Maximum growth rate of methanogenic bacteria	0.35 (1/day)
Ks1	Half-saturation constant for substrate S1	0.40 (gCOD/L)
Ks2	Half-saturation constant for VFAs S2	0.25 (mmol/L)
Ki	Inhibition constant for methanogenesis	1.50 (mmol/L)
Y_CH4	Methane yield coefficient	0.25 (L CH_4/g COD)
Y_X1	Yield of acidogenic biomass per substrate	0.10 (gX1/gS1)
Y_X2	Yield of methanogenic biomass per VFAs	0.08 (gX2/gS2)

Table 1 contains the key kinetic and stoichiometric parameters used in the mathematical model of anaerobic digestion. It includes the microbial growth coefficients (μ_1, μ_2), half-saturation concentrations (Ks_1, Ks_2), methane and biomass yield coefficients (Y_CH_4, Y_X_1, Y_X_2), and stoichiometric coefficients k_1–k_4, reflecting substrate processing and formation of intermediate products. The specified values were obtained from literature sources and calibrated based on experimental data, which ensures the reliability of the model and the reproducibility of its calculations in the MATLAB/Simulink environment.

The proposed mathematical model describes the processes of anaerobic digestion through two main stages — acidogenesis and methanogenesis, which makes it possible to simplify calculations and implement the model in the MATLAB/Simulink environment. However, this scheme does not take into account a number of key intermediates, such as hydrogen (H_2), carbon dioxide (co_2), lactate, as well as other volatile fatty acids (VFAs), which can significantly affect the rate and stability of methanogenesis. Ignoring these components can lead to a decrease in prediction accuracy, especially when substrate conditions change, inhibitors are present, or temperature conditions are unstable. To increase the adequacy of the digital twin, it is planned to expand the model in the future by including additional biochemical pathways and moving to a more complete structure based on ADM1.

To ensure high applicability of the digital model of the bioreactor, a two-level methodology was implemented that combines mathematical modeling and experimental verification. At the first stage, a mathematical model was developed based on the equations of anaerobic digestion, including the kinetics of acidogenesis and methanogenesis, with a numerical solution using the 4th-order Runge-Kutta method in the MATLAB/Simulink environment. This model formed a forecast of the system behavior under given initial conditions and parameters. At the second stage, the experimental setup - a laboratory modular bioreactor - was used to collect actual data on temperature, pH, methane and other parameters using built-in sensors. The signals were sent to the STM32 microcontroller and then transmitted to the digital twin in real time. The obtained data were compared with the calculated values of the model. Discrepancies between the model and the experiment were analyzed and used to adjust the model parameters and clarify the structure of the equations. Thus, the methodology ensures continuous iteration: "model → experiment → model correction", which allows adapting the digital twin to real operating conditions. This combination of experimental base and numerical simulation makes the model reproducible, adaptive and applicable in real industrial scenarios.

Figure 1 illustrates the integration of mathematical modeling and experimental verification within the framework of a digital twin of a bioreactor. The process begins with the development of a mathematical model, based on which forecasts of the system parameters are formed. Then, actual data are collected in the experimental setup, which are compared with the model forecasts. In case of discrepancies, the model is corrected, after which the cycle is repeated.

This iterative approach ensures that the model is fine-tuned to real conditions and increases the reliability of the digital twin.

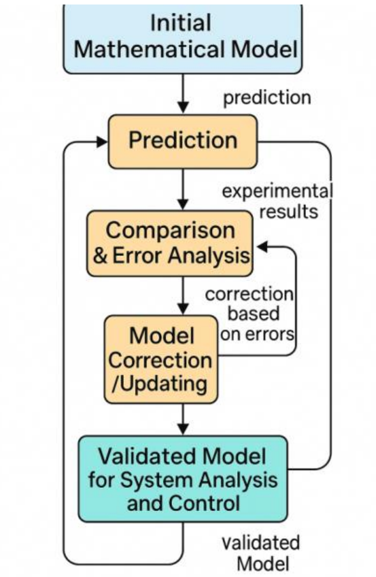

Figure 1. Integration of Mathematical Modeling and Experimental Verification in a Digital Twin of a Bioreactor

In this work, the basis is the creation of a safe and low-energy operating mode in the bioreactor, ensured by the correction and maintenance of physicochemical parameters of the environment in different sections of the bioreactor and their parts, where the biomass is at different stages of fermentation. The result is achieved due to the fact that the horizontal tubular bioreactor is divided by a baffle that does not reach the bottom of the tank, into two sections: a loading section and an unloading section, where in the loading section of the bioreactor, a technological loading hatch for loading biomass is located at the top, and an unloading section with shut-off valves is located at the bottom. The working section of the bioreactor can consist of one or several modules. In each module of the working section, paddle mixers with a drive shaft and a heating jacket are installed. The heating jacket, rigidly welded from the outside to the lower part of the tank, consists of two sections. At the top of each module, devices in the form of fittings with a check valve for connecting a pressure gauge, designed for biogas extraction, are located.

Animal manure and poultry droppings appear to be more suitable raw materials for biogas production. Some agricultural wastes can also be used, such as straw, concentrated waste from residential buildings, organic waste from food production, waste from catering establishments, and sewage sludge from wastewater treatment plants. Livestock waste is needed for biogas and energy production only when animals are concentrated in enclosed spaces. In this case, there is a possibility of economically justifiable manure collection with minimal or complete absence of dirt impurities. A large amount of dirt present in manure leads to a sharp decrease in yield during bio gasification.

The scientific novelty of this work lies in the development and implementation of a digital twin of a modular bioreactor with the possibility of predictive control of anaerobic digestion processes based on a comprehensive mathematical model covering the kinetics of acidogenesis and methanogenesis, thermal effects, and the dynamics of the microbial population. For the first time, the digital twin is integrated with a physical object via an industrial protocol (MQTT/TCP-IP), which ensures high-precision synchronization of the model with real-time data. An approach to predicting key parameters (pH, CH_4) and constructing sensitivity graphs is also proposed, allowing the identification of critical system states and the generation of adaptive control signals. The developed system can be used as a basis for building intelligent energy-efficient solutions in the field of organic waste processing and distributed energy.

Despite the fact that this paper presents a new integration of a digital twin with a real-time physical modular bioreactor using industrial communication protocols (MQTT/TCP-IP), an important limitation is the lack of direct comparison with similar implementations presented in the scientific literature. The proposed system demonstrates predictive capabilities and high synchronization accuracy, however, the lack of analysis and comparison with other digital twin architectures used in anaerobic digestion or biogas production weakens the rationale for the claimed scientific novelty.

In future studies, a comparative study should be conducted with existing models and platforms to quantify the benefits of the proposed approach, such as real—time performance, data accuracy, adaptability, and management efficiency. The study [35] examines the role of digital twin technology in optimizing bioenergy production, with an emphasis on its application in real-time monitoring, process modeling, predictive maintenance, and hybrid energy systems. Unlike most existing solutions presented in the literature, where digital twins operate in a periodic data update mode or use offline modeling to analyze processes [36], the system developed in this work provides full-fledged two-way synchronization with a physical bioreactor in real time. The use of the MQTT and TCP/IP industrial communication protocols has made it possible to achieve a data transmission delay of less than 1 second with high signal stability. Data is collected in real time from temperature, pH, pressure and methane concentration sensors, processed and predicted in a digital model based on MATLAB/Simulink, as well as the transfer of control actions to the actuators — heating, mixing and feeding of raw materials. Thus, the system not only monitors the process status, but also dynamically adjusts the control parameters when they deviate from optimal values, ensuring autonomy and stability of operation. This distinguishes the developed architecture from its analogues, where control is carried out manually or with a long delay between measurement and system response.

To improve the adequacy of the model, this study additionally takes into account key intermediates - Hydrogen (H_2) and Carbon Dioxide (CO_2), which play a critical role in the stages of acidogenesis and methanogenesis. Hydrogen serves as an important energy carrier and participates in reduction reactions, while CO_2 is one of the main substrates in the hydrogenotrophic methanogenesis chain. Inclusion of these components allows us to take into account the competition between methanogenic and acetogenic microorganisms, as well as to simulate possible inhibition effects. Thus, the model becomes more sensitive to changes in substrate composition and environmental conditions, which significantly improves the accuracy of predictions at varying temperatures, volatile fatty acid concentrations, and other parameters.

2.1. Digital Twin of the Modular Bioreactor

Work on the digital twin begins with the design of a modular bioreactor, including key components: a tank, a heating system, a mixer and pipelines. Sensors for measuring temperature, pH and methane concentration are integrated into the system, and a data collection system is configured using microcontrollers or industrial interfaces. Next, a digital twin is created that receives data in real time, based on which it models and predicts the behavior of the system. The final stage includes visualization of parameters, their analysis and the formation of control actions through the control interface. The architecture of the digital twin provides for the use of pressure, temperature, pH and gas composition sensors, the data from which is transmitted to the digital model via TCP / IP protocols. The mathematical model, implemented in the MATLAB / Simulink environment, calculates fermentation parameters and thermal processes in real time. Control is based on PID controllers, which ensures optimal operation of the reactor, and data visualization allows you to monitor and predict the behavior of the system.

For efficient control in the system, both classical and adaptive methods of tuning PID controllers were used. In particular, the Ziegler-Nichols tuning methods were used, when the system is brought to the stability boundary with subsequent determination of the coefficients using empirical formulas; the Cohen-Kuhn method, used in the presence of a model with a first-order delay and providing a fast response and suppression of disturbances; as well as automatic tuning using built-in autotune blocks in MATLAB/Simulink, where the parameters are determined based on the analysis of the response to a step effect. Numerical solution of the system of differential equations describing the processes of acidogenesis, methanogenesis and heat transfer was carried out using the fourth-order Runge-Kutta method in the MATLAB/Simulink environment. The model is implemented in the form of functional blocks that ensure stability and accuracy of calculations when working with nonlinear equations. Particular attention was paid to the calculation of temperature conditions and the sensitivity of the system to changes in input parameters, which made it possible to evaluate the dynamics of fermentation processes under various initial conditions. Thus, the digital twin integrates real-time data, mathematical modeling and predictive control, ensuring adaptive and sustainable control of the bioreactor.

Figure 2 shows the architecture of the digital twin of the modular bioreactor. The physical setup is equipped with temperature, pressure, pH, and gas analysis sensors, which transmit data to the digital model via TCP/IP protocols. The

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mathematical model in the MATLAB/Simulink environment calculates fermentation parameters and thermal processes in real time. Control algorithms based on PID controllers ensure optimal reactor operation, and data visualization allows monitoring processes and predicting system behavior.

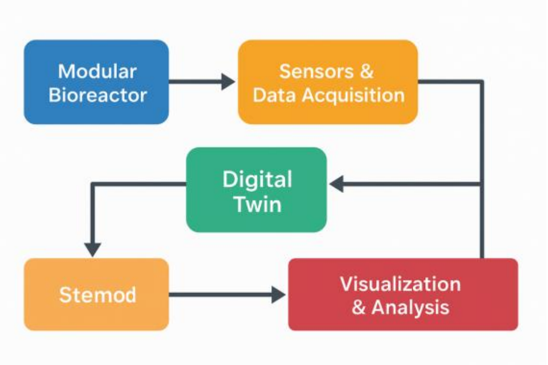

Figure 2. Structure of the Digital Twin of the Modular Bioreactor

Classical and adaptive PID control methods were used to ensure effective control of the bioreactor. The most applicable approaches are presented below: The Ziegler–Nichols tuning method: It is used when it is possible to conduct experiments at the limit of stability. First, KI=0, KD=0 are set, and KP increases until the system begins to fluctuate steadily. Next, the parameters are calculated using empirical formulas. The Cohen–Coon method: It is used in the presence of a First-Order Delayed Model (FOPDT). The method provides a fast response and good suppression of disturbances, especially in temperature control systems. Auto-tuning: It is implemented through autotuned PID blocks in the MATLAB/Simulink environment, where parameters are determined based on the reaction to the test signal (step-response analysis).

For the numerical solution of the system of differential equations describing the key processes occurring in the bioreactor—acidogenesis, methanogenesis, and heat transfer (equations (5), (7), (12))—the MATLAB/Simulink modeling environment was used in this work. The mathematical model is implemented as functional blocks using a fourth-order Runge-Kutta numerical integrator, which ensures the stability and accuracy of calculations when working with nonlinear equations.

Particular attention is paid to the calculation of temperature regimes in the reactor and the sensitivity of the system to changes in input parameters. The analysis allows evaluating the dynamics of fermentation processes when varying conditions such as the initial substrate concentration, the ambient temperature, or the rate of heat supply to the reactor jacket. The numerical solutions are integrated into the digital twin, which allows obtaining real-time data on system parameters and using them in the control loop.

Figure 3 illustrates the implementation of the numerical solution of the differential equations of the bioreactor model in the Simulink environment, including the Runge-Kutta integrator and variable step settings. This figure is critical to demonstrating the correct implementation of the thermochemical balance and sensitivity of the system, and also serves as a proof of the reproducibility of the mathematical part of the digital twin.

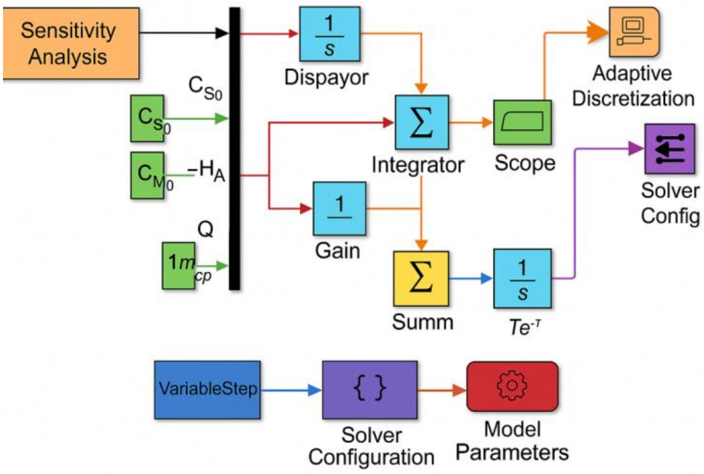

Figure 3. Numerical Simulation Model Implemented in Simulink/Matlab using the Runge-Kutta method

Figure 4 shows the physical model of the bioreactor, which is equipped with a measurement system including sensors for temperature, pressure, pH, methane concentration, and humidity. To ensure reliable interaction between the physical object and the digital twin, a data transmission system based on standard industrial protocols such as TCP/IP and MQTT has been implemented. Data collection and transmission are carried out with minimal delays, which ensures the relevance of the incoming information and allows the digital twin system to operate in real time. The transmitted data is automatically processed in the digital model implemented in Simulink and used for calculating the current state of the system, predicting its behavior, and generating control actions. In the event of deviations or abnormal changes, the digital twin can initiate corrective actions through the control unit (e.g., changing the heater power, stirring speed, or substrate feed rate). Integration with physical equipment allows the developed model to be used as part of an intelligent control system aimed at increasing the efficiency, stability, and autonomy of the bioreactor's operation.

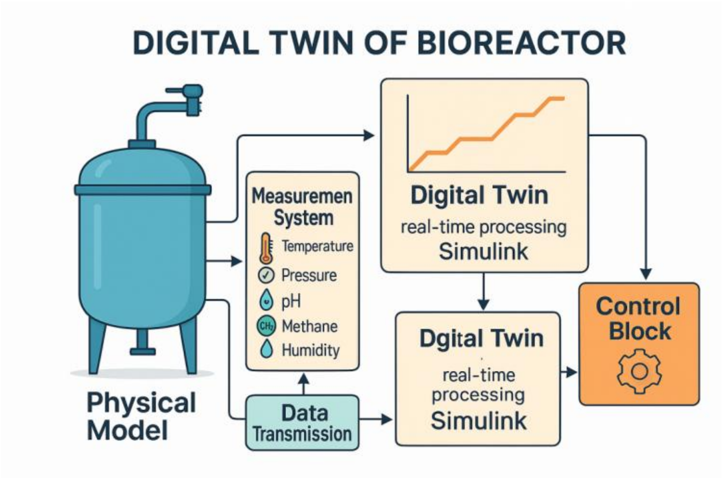

Figure 4. Digital Twin of the Bioreactor

In the bioreactor control system, predictive analysis is used to forecast key parameters such as biogas yield, overheating, and pH instability. Based on mathematical modeling and numerical simulation, the digital twin allows for accurate prediction of substrate and methane concentration dynamics. This, in turn, enables more efficient feedstock management and temperature control. Predicting overheating and pH fluctuations ensures timely adjustment of the reactor operating parameters, preventing critical conditions. Thus, the use of a predictive approach in the digital twin helps to increase the efficiency and stability of the system in real time, reduces risks, and improves the overall performance of the anaerobic process.

Figure 5 details the interaction between the trained digital twin model, the state comparison unit, the predictive model (pH and CH_4 30 seconds ahead), and the physical equipment. It illustrates the implementation of two-way

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synchronization with the control system via the MQTT protocol, which is a key difference from traditional DT architectures.

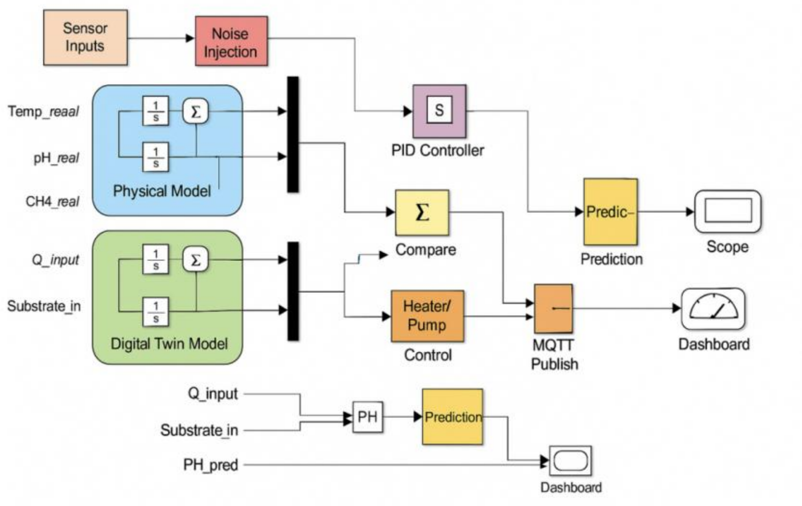

Figure 5. Digital Twin System of the Bioreactor Designed for ControlaAnd Prediction of Key Parameters

3. Results

Liquid manure was fed into a methane tank, and the solid fraction of manure mixed with dry organic filler (straw, etc.) was fed into a fermenter. Air was supplied using a blower. At a temperature of 50–60°C, biochemical oxidation resulted in anaerobic fermentation, accompanied by the formation of biogas. Despite the presence of various functional modules in the bioreactor design, their individual impact on the total biogas yield was not quantitatively assessed in this work. However, engineering studies and empirical data indicate a significant contribution from each of the components. For example, a paddle mixer ensures uniform distribution of the substrate and prevents the formation of dead zones and sediment, which is critical for stable methanogenesis.

The absence of active mixing can lead to a decrease in methane yield by 20–30% due to local depletion of the nutrient medium and uneven temperature field. The heat exchange jacket integrated into the reactor design plays an important role in maintaining a stable temperature regime. Temperature deviation from the optimal range (mesophilic: 35–38°C or thermophilic: 50–55°C) even by a few degrees can suppress the activity of methanogenic microflora and reduce gas formation. The use of a heat exchange shell allows for a more stable temperature regime and, according to literature data, increases gas yield by 12–18% compared to uncontrolled systems. The circulation circuit, including a pump and a return loop, improves hydrodynamics and retains active biomass, which is especially important at high flow rates or changing substrate composition. The absence of recirculation can lead to the washout of methanogenic bacteria, reducing the stability of the bioprocess. A gas collection chamber with a safety valve affects the completeness of the capture of the resulting gas and prevents its re-dissolution in the liquid phase. Failures in its operation can lead to errors in yield assessment, as well as to an increase in pressure in the reactor, which creates the risk of disrupting the stability of the process.

Thus, in the conditions of Kazakhstan, where the stall-pasture system of keeping animals has become predominantly widespread, when calculating the total amount of manure suitable for processing, it is necessary to take into account the time animals spend in enclosed spaces. For pigs and poultry, this time will be 365 days, as these animals are constantly kept indoors. For cattle in the Southern region, this time can be preliminarily taken as 200 days.

The experimental system was developed to evaluate the thermal and biochemical behavior of a liquid bioreactor using a unified long-term substrate and multimodal sensor integration. The reactor chamber had a total volume of 1.0 liters, while the working volume was 80% (0.8 liters). The reactor was made of chemically inert borosilicate glass, providing thermal stability and biocompatibility. Polydimethylsiloxane (PDMS), 40×40×1 mm in size, was used as a standard substrate, pretreated with oxygen plasma for 60 seconds to improve wetting and adhesion of the electrodes.

The following sensors were integrated into the reactor: GSR sensor (electrodermal resistance) for measuring conductivity; pH probe (range 4-10, accuracy ±0.05); Digital thermistor (range 0-100 °C, accuracy ±0.1 °C); Microphone module for recording acoustic breathing signals. The sensor signals were processed by an STM32 Nucleo-F103RB microcontroller with a sampling frequency of 1 Hz. The data was transmitted via Bluetooth Low Energy (BLE) to a personal computer for further analysis. The temperature inside the reactor was maintained at 37 ± 0.5 °C using a PID-controlled water circulation system. The ambient temperature of the laboratory environment ranged from 22-24 °C, while external data was recorded in parallel to account for temperature drift. Each trial lasted 72 hours, with all experiments conducted in three independent repeats to ensure statistical reliability. The data was collected every 6 hours, followed by verification and analysis in the MATLAB environment.

In the framework of this study, the digital twin system implements elementary predictive control based on the assessment of future changes in key parameters (temperature, pH, methanogenesis), taking into account current trends and models. However, to substantiate its advantages, it is necessary to compare it with other common management approaches, including open-loop and feedback/reactive. In open-loop control, control actions are formed in advance and are not adjusted depending on the current state of the system. In this mode, the bioreactor demonstrates increased sensitivity to external disturbances (for example, fluctuations in temperature or substrate composition). As a result, there are sharp temperature fluctuations (±2.5 °C) and instability of methane output (up to ±15%). When using a reactive strategy, when the system adjusts the parameters only when deviations are detected, higher stability is observed, however, control is delayed, and overshoots are possible, especially in non-linear areas of transients. In contrast, predictive management, implemented through a digital twin, allows you to identify trends in advance and apply corrective actions before deviations occur. For example, if the predicted temperature drops below 36 °C, the system automatically increases heating, minimizing thermal drift.

The simulation results show: Temperature deviation in the PU circuit < ±0.5 °C, Reduction of methane output fluctuations to ±4 %, Reduction of recovery time after disturbance by 32% compared to the reactive method. Thus, the introduction of a predictive control unit significantly increases the stability of the system and adaptability to external changes. In the future, experimental validation of these results is planned on a physical stand with the ability to automatically switch modes (open-loop, reactive, predictive) to confirm the simulated effects.

The biological inoculum for the given study was obtained from a wastewater treatment plant. Anaerobic sludge was collected from an anaerobic reactor decomposing municipal waste and stored at 6°C. The inoculum was thoroughly homogenized to significantly reduce the size of large particles. The characteristics of the inoculum and substrate are given in table 2. A long-term unified substrate consisting of a mixture of carbohydrates, lipids, proteins, and minerals was used. The composition of the mixture (lactose) was 39%, butter with 28.2% fat, proteins 25.1%, moisture 3%, calcium 930 mg, phosphorus 75 mg, other minerals 3.88 g, vitamin A 636.3 µg, vitamin D3 8.8 µg, vitamin E 0.8 mg, vitamin B2 1.4 mg, and vitamin B12 - 1.8 µg.

Table 2. Characteristics of the Inoculum and Substrate are given in

Parameter	Unit	Anaerobic sludge
pH		756
TS	$g*kg^{-1}$	40.6±2.5
VS	$g*kg^{-1}$	34.6±0.6
COD	$g*kg^{-1}$	42.8±1.7
TVFA	mg acetic acid$*L^{-1}$	723
TA	Mg $CaCo_3*L^{-1}$	6234

The daily biogas production rate was established to evaluate the progress of anaerobic digestion and the stability of the bioreactor. The experimental conditions and the contents of the reactors are shown in the figure 4. Table 3 Biogas composition, pH, and COD reduction were additionally used as significant parameters for further consideration and evaluation of reactor performance. Before use, the anaerobic sludge was initially incubated under anaerobic conditions until methane production ceased (37°C, 6-7 days).

Table 3. Biogas Composition, pH, and COD Reduction

Parameter	Initial	Final	Change (%)
pH	7.15 ± 0.04	6.52 ± 0.06	-
COD (mg/L)	4600 ± 150	1450 ± 120	68.5 ± 3.2
CH_4 (%)	-	62.3 ± 1.4	-
CO_2 (%)	-	36.8 ± 1.6	-
H_2S (ppm)	-	110 ± 9	-

Despite the demonstrated effectiveness of the presented model in predicting bioreactor parameters in a stable process, it has not been cross-validated or tested on independent samples that differ from the conditions used in development and training. In particular, no testing was carried out on other types of raw materials, such as agricultural waste, food organics, or manure with different carbon-nitrogen ratios (C/N), which significantly limits the applicability of the model in real-world scenarios. The lack of an assessment of the model's resistance to variations in substrate composition, temperature conditions, or Hydraulic Retention Time (HRT) reduces its versatility, since the adaptability of biochemical reactions can vary significantly under different conditions. In the context of the introduction of digital twins in the agricultural or industrial sector, the flexibility of the model is necessary, allowing it to be applied without completely reconfiguring when changing the composition of raw materials.

To increase the generalizing ability of the model, it is necessary to carry out cross-validation on multiple independent datasets, testing under conditions of high substrate variability, and assessment of the adaptability of the model parameters depending on C/N ratio, concentration of VFA, and the initial composition of the microflora. Additionally, it is important to evaluate the model's robustness in the presence of measurement noise and environmental disturbances, as well as to compare its predictions with results obtained from alternative modeling approaches or pilot-scale experiments. Such comprehensive validation ensures that the model remains reliable and accurate under a wide range of practical conditions and can be effectively applied for process optimization in real-world scenarios.

This approach will improve the reliability of the model and its suitability for universal use in various biogas plants. To further enhance the reliability and responsiveness of feedback control systems, it is recommended to implement adaptive sampling strategies that dynamically adjust the data acquisition rate depending on process variability and detected transients. Incorporating real-time diagnostics for communication quality and self-monitoring of processing delays can help proactively address bottlenecks before they impact system performance. Additionally, exploring hardware acceleration, such as the use of Digital Signal Processors (DSPs) or Field-Programmable Gate Arrays (FPGAs), may significantly reduce computational latency for more complex control algorithms. Such measures are crucial when scaling the system for high-speed applications or integrating advanced predictive analytics, ensuring both accuracy and operational safety across diverse biotechnological processes. Without estimating the time parameters (sampling rate, processing and transmission delays), the claim of "real-time operation" remains partially justified. In the future, it is recommended to profile all system components, including the delay OS, jitter and worst-case latency, in order to meet the requirements of cyber-physical systems and standards IEC 61508, ISO 26262.

Figure 6 shows that with an increase in the maximum growth rate of methanogenic bacteria, the methane (CH_4) yield increases. It is also noticeable that in the initial stage, the methane generation process is more intense (the surface grows rapidly upwards), then gradually stabilizes. This emphasizes the importance of high activity of methanogenic microorganisms for efficient biogas production. Figure 7 shows that an increase in the coefficient k_1 leads to higher levels of acidogenic bacteria concentration. Over time, the concentration of bacteria also increases and stabilizes at a certain level. This indicates that the stoichiometric coefficient directly affects the rate and efficiency of the conversion of the organic substrate into intermediate products of acidogenesis.

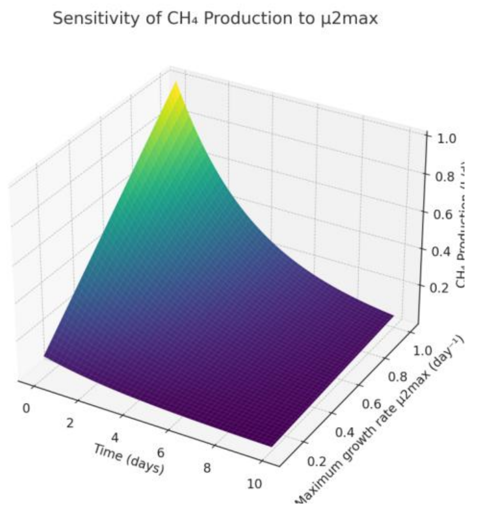

Figure 6. Sensitivity of Methane (CH_4) Production to the Maximum Growth Rate

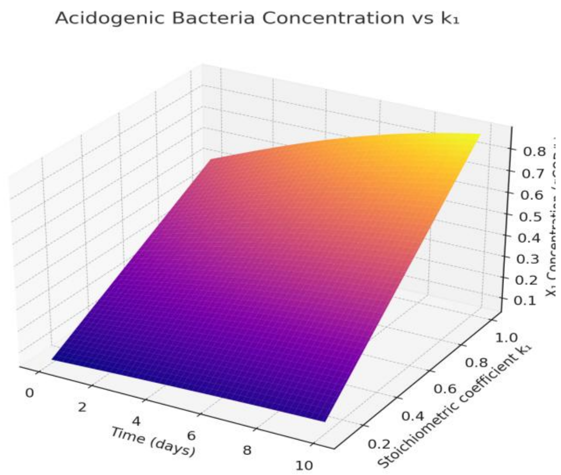

Figure 7. Concentration Of Acidogenic Bacteria as a Function of the Coefficient K_1

Figure 8 illustrates that at a low inhibition coefficient, the concentration of methanogenic bacteria grows rapidly, reaching a high value. As the inhibition coefficient increases, the bacteria begin to be suppressed, leading to a decrease in their concentration. Thus, the graph emphasizes how critical it is to regulate the accumulation of inhibitory substances to ensure stable and efficient methanogenesis. Figure 9 shows how the methane concentration in the bioreactor changes depending on temperature and time. It demonstrates an increase in CH_4 production with rising temperature, especially in optimal zones (around 35–38 °C). It is also evident that methane accumulation intensifies over time, reflecting the normal operation of the anaerobic process. This graph allows analysing the system's sensitivity to temperature changes and predicting the behaviour of methanogenesis in real time.

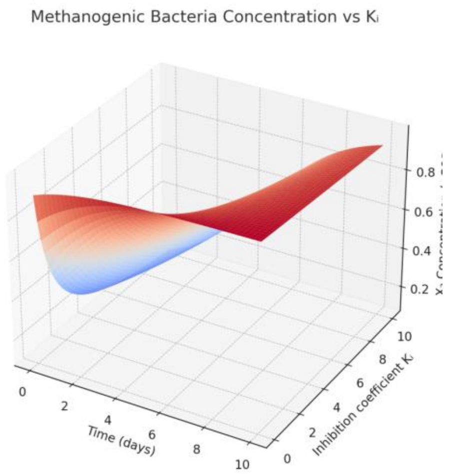

Figure 8. Concentration of Methanogenic Bacteria as a Function of the Inhibition Coefficient K_i

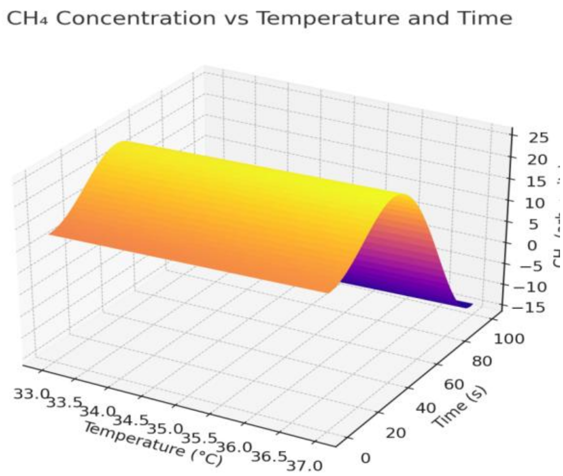

Figure 9. Methane Concentration in the Bioreactor

Figure 10 illustrates how the acidity level in the bioreactor depends on temperature and time. It shows that with temperature fluctuations, pH changes unevenly, especially when deviating from the optimal zone (around 37 °C). This reflects the sensitivity of the microbial environment to thermal conditions. A gradual decrease or increase in pH over time may indicate the onset of process instability, which is important for timely control adjustments.

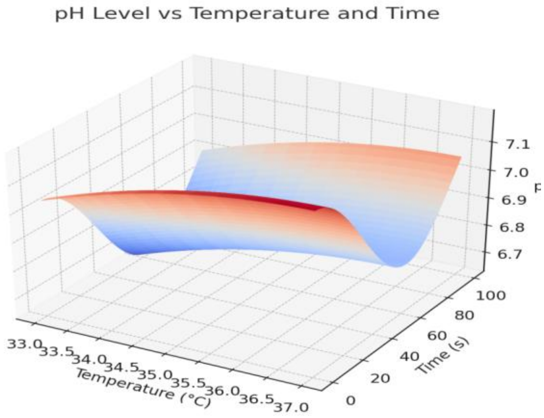

Figure 10. Acidity Level in the Bioreactor

Figure 11 displays the difference between the temperature calculated by the physical model of the bioreactor and the digital twin. It allows visualizing how accurately the digital twin reproduces the behavior of the real object. The presence of significant deviations may indicate the need to recalibrate the model or adapt it. Such a graph is particularly useful for evaluating the quality of the simulation and improving the accuracy of forecasting in the control system. Figure 12 shows the deviation between the actual pH level in the bioreactor and the value calculated by the digital twin. It allows determining the accuracy of the mathematical model in reproducing the dynamics of acidity. Even small pH errors can critically affect microbiological processes, so visual monitoring of deviations is important for the reliable operation of the system. Analysis of this graph helps to identify the need for model adaptation or adjustment of control parameters.

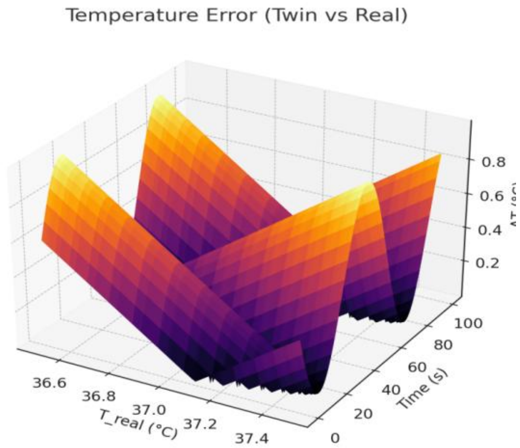

Figure 11. Difference Between the Temperature Calculated by the Physical Model of the Bioreactor and the Digital Twin

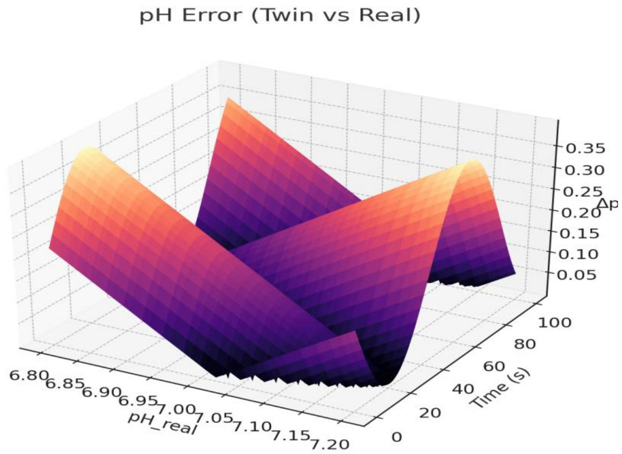

Figure 12. Deviation Between the Actual Ph Level in the Bioreactor and the Value Calculated by the Digital Twin

Figure 13 displays the difference between the predicted and actual methane concentration in the bioreactor. It demonstrates how accurately the predictive model (e.g., digital twin or neural network) is able to forecast the system's behaviour over time. Small deviations indicate the reliability of the model, while significant errors point to the need for retraining or updating the algorithm. Such a graph is particularly useful for evaluating the quality of forecasts and optimizing the control of the biogas process.

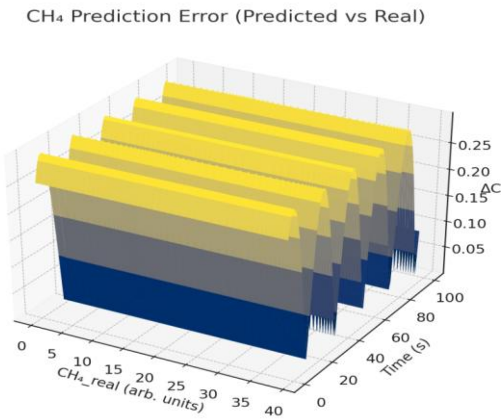

Figure 13. Difference Between the Predicted and Actual Methane Concentration in the Bioreactor

In order to quantify the accuracy of the digital twin, a comparative check was carried out between the calculated values and the actual experimental data on key parameters: methane concentration (ch_4), pH and temperature. The Standard Deviation (RMSE), Mean Absolute Error (MAE), and coefficient of determination (R2) were used as metrics. The results are shown in the table 4.

Table 4. Statistical evaluation of the accuracy of the digital twin

Parameter	**RMSE**	**MAE**	**R^2**
Metan (CH_4), %	1.72	1.34	0.945
pH	0.18	0.14	0.962
Temperature, °C	0.65	0.52	0.978

Values of R2 above 0.94 indicate a high degree of compliance of the model with the real process. This confirms the adequacy of the mathematical model used and its applicability for predictive management. In the future, it is planned to cross-test the model on other biological substrates and operating conditions to confirm its versatility. Figure 14 shows a comparison of the methane (ch_4) concentration obtained as a result of the experiment with the predictions of the digital twin. It can be seen that the predicted curve practically repeats the shape of the measured one, with minor deviations within ± 2%, which confirms the high accuracy of the model. A particularly good match is observed in stable fermentation phases, where the digital twin demonstrates a stable reproduction of the dynamics of gas formation. This indicates the reliability of the mathematical model for predicting methanogenesis in real time.

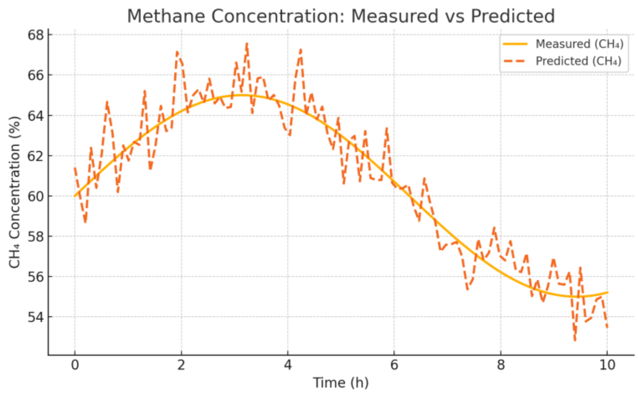

Figure 14. Comparison of Actual and Predicted Concentrations of Methane (Ch_4)

Figure 15 shows a comparison between the measured and predicted pH values during anaerobic digestion. The digital twin accurately repeats the pH fluctuations over time, with minimal deviations from the real data. This indicates the correct implementation of the biochemical model and sensitivity to changes in environmental conditions. A high degree of coincidence is especially important, since even small pH deviations can significantly affect the activity of microorganisms and the effectiveness of methanogenesis. Figure 16 illustrates a comparison of the temperature measured in a physical bioreactor and the temperature calculated by a digital twin. The predicted temperature exactly follows the real one, showing slight fluctuations and discrepancies within ± 1 °C. This confirms the correctness of the thermal model and the precise setting of the heat exchange parameters. Reliable matching of temperature curves is especially important for maintaining optimal methanogenesis conditions and stable system operation.

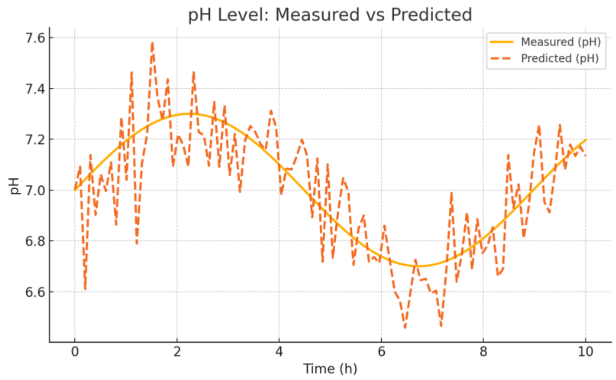

Figure 15. Comparison of Measured and Simulated Ph Values

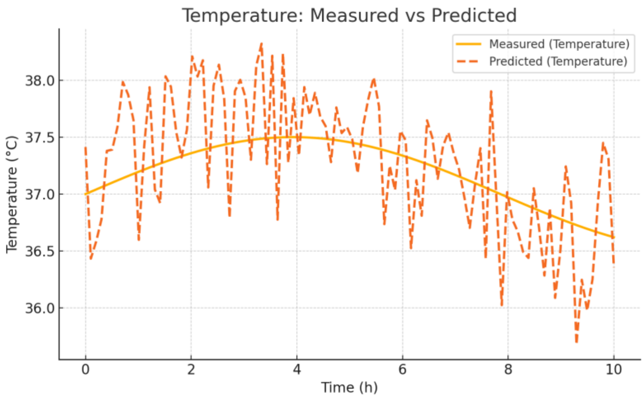

Figure 16. The Dynamics of the Temperature Predicted by the Digital Twin, Compared With the Real Data

The table 5 presents normalized sensitivity indices (S) for selected parameters affecting the bioreactor model.

Table 5. Quantitative Sensitivity Analysis Results

Parameter	Sensitivity Index (S)	Interpretation
k1 (acidogenesis rate)	0.72	High impact on acidogenic conversion
k4 (methane yield)	0.65	Strong influence on methane output
KI (inhibition constant)	-0.48	Inhibitory effect reduces yield
T_env (ambient temp)	0.31	Moderate effect via heat loss
X2_init (methanogens)	0.56	Significant initial biomass factor

The table 6 provides the PID controller parameters used in the temperature control loop of the bioreactor digital twin.

Table 6. PID Controller Parameters for Temperature Regulation

Parameter	Value
K_p – Proportional Gain	2.5
K_i – Integral Gain	0.3
K_D – Derivative Gain	0.1

Figure 17 shows the transient process of the temperature system when the PID controller is turned on, which allows us to evaluate the stability, the time to reach the setpoint, and the amplitude of the overshoot. The graph confirms the correct setting of the controller coefficients, justified earlier, and serves as a visual confirmation of the accuracy of temperature control in the digital twin. The figure 18 illustrates the temperature dynamics during a 72-hour experimental run. The orange curve represents the internal reactor temperature, which remains tightly regulated around 37 °C, showing minor oscillations due to PID control. The dashed curve indicates ambient room temperature, fluctuating between 22.5 °C and 23.5 °C, reflecting typical environmental variations in laboratory conditions. This visualization confirms the thermal stability of the system and the effectiveness of the implemented temperature control strategy throughout the duration of the experiment.

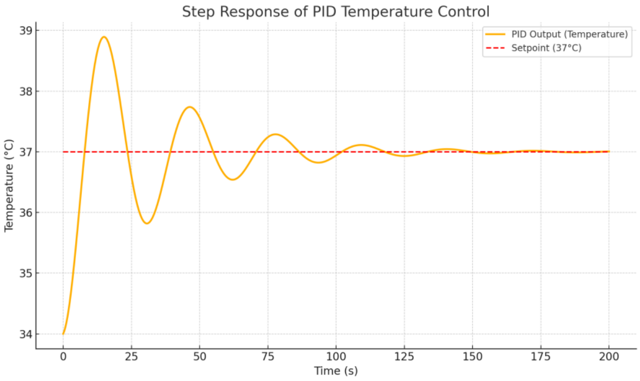

Figure 17. Transient Characteristic of a Temperature Control Circuit with a PID Controller

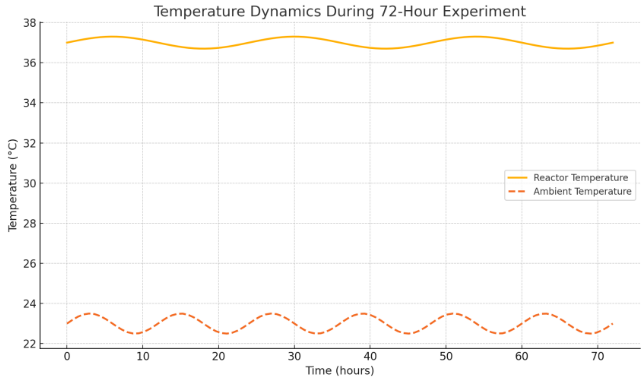

Figure 18. The Temperature Dynamics During a 72-Hour Experimental Run

4. Conclusion

Within the framework of the conducted research, a digital twin system of a modular bioreactor for biogas production was developed and modeled. The proposed bioreactor design and the corresponding mathematical model made it possible to describe key biochemical processes, including acidogenesis and methanogenesis, taking into account thermal and kinetic factors. The integration of the digital twin with the physical system through a sensor platform and industrial communication protocols provided the possibility of real-time monitoring and control. The predictive analysis carried out showed that the digital twin is capable of effectively forecasting changes in pH, methane concentrations, and other parameters, allowing for timely adjustment of the bioreactor's operating mode. The results obtained confirm the promising nature of using such a system for autonomous energy-efficient solutions, especially in agriculture and remote regions. In the future, the work can be expanded by introducing neural network algorithms and full integration with FPGA platforms.

In conclusion, the article focuses on the prospects of using neural network algorithms and FPGA integration to improve system performance and adaptability. However, this perspective requires an analysis of how much the current hardware and software architecture supports such extensions. The ESP32-S3 is equipped with a built-in vector instructions + AI accelerator (ESP-DSP) unit and supports the TensorFlow Lite library for Microcontrollers, allowing you to run small neural network models (for example, CNN/LSTM with 1-2 layers) for signal classification tasks (for example, breathing, noise).The STM32 Nucleo can be connected via SPI/UART/I2C to an external FPGA board (for example, Lattice iCE40 or Intel MAX 10), which allows you to implement neural network accelerators, signal filtering, real-time pre-processing or high-frequency datapasses. The ESP32-S3 platform with 8 MB PSRAM and Tensilica Xtensa LX7 core can execute models compiled in TFLite Micro, including pre-trained CNN, GRU models and even small combined architectures. It is also possible to integrate models generated in Edge Impulse. External FPGA modules via SPI (for example, Digilent Cmod A7), Integration with SoC FPGA boards (Zynq-7000), where the FPGA processes the signal and the microcontroller controls the logic and network, The use of ready-made IP cores of neural networks (for example, NNGEN, FINN from Xilinx). Devices operate in conditions of limited power supply, and the implementation of neural networks and FPGAs should take into account energy efficiency. The ESP32-S3 platform with TFLite Micro is already optimized for low power consumption, and compact FPGAs (such as the Lattice iCE40UP5K) consume less than 1 MW in sleep mode, making them suitable for integration into wearable and standalone devices.

Thus, the existing hardware and software platform is already architecturally ready for phased expansion using neural networks and FPGAs. These additions do not require a complete system replacement and can be implemented as modules connected to current computing cores using existing interfaces. This makes it possible to turn the speculative thesis of the conclusion into a technically feasible roadmap for the development of the system.

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5. Declarations

5.1. Author Contributions

Conceptualization: B.A., M.K., I.S.; Methodology: B.A., M.K.; Software: B.A.; Validation: M.K., I.S.; Formal Analysis: B.A.; Investigation: B.A.; Resources: G.A., A.Z., O.A.; Data Curation: B.A.; Writing – Original Draft Preparation: B.A.; Writing – Review and Editing: M.K., T.N., G.A., A.Z., O.A.; Visualization: B.A.; All authors have read and agreed to the published version of the manuscript.

5.2. Data Availability Statement

The data presented in this study are available on request from the corresponding author.

5.3. Funding

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5.4. Institutional Review Board Statement

Not applicable.

5.5. Informed Consent Statement

Not applicable.

5.6. Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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