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OPTIMIZING BIOGAS PRODUCTION USING ARTIFICIAL NEURAL NETWORK

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The object of this study is the operating parameters of the anaerobic digestion unit. The study aims to increase the potential of biogas production. The task to select the optimal parameters of the working process of anaerobic digestion has been solved.

A model of cumulative biogas and methane output in the process of anaerobic waste digestion has been constructed, which is conceptualized using the method of artificial neural network. The model is built on the basis of 11 process-related variables, such as hydraulic retention time, pH, operating temperature, etc.

The plant parameters, leading to the highest volume of biogas production, were selected. It was determined that the optimal amount of biogas can be brought to 90 %, which exceeds the maximum value obtained from factory records by 12.6 % to 700 m^3/t. Working conditions that led to optimal methane production were defined as the temperature of 39 °C, the total solids of 4.5 %, the organic percentage of 97.8 %, and pH 8.0.

It was found that biogas production is the highest at temperature within the thermophilic range while the local maximum is achieved in the mesophilic temperature range.

The model built serves to determine the optimal operating parameters for maximum biogas production and could be used to optimize biogas production productivity using limited experimental data. The model also makes it possible to predict the performance of anaerobic digestion under untested conditions.

It is possible to practically use the developed biogas production model when monitoring the operation of the anaerobic digestion unit, to increase the efficiency of the process, and when adjusting the working conditions of the methane tank

Keywords: biogas plant, artificial neural network, biogas yield potential, anaerobic digestion

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1. Introduction

Every year the urgent problem of the shortage of fossil fuel and energy resources is exacerbated. One of the ways to overcome it is to diversify energy production through alternative sources.

Special attention in this context should be paid to the method of obtaining biomethane at biogas plants or anaerobic digestion (AD) plants, as a promising direction in the fuel and energy sector.

Biogas production accounts for only about 8 % of total renewable energy production in the European Union [1]. In general, biomass energy occupies a relatively small segment of renewable energy. However, the biogas market shows a stable exponential nature of growth of 450 %. In addition, it is one of the fastest growing markets [2]. The number of biogas plants in Europe is steadily growing and in 2015 amounted to 17376 installations, which corresponds to 8728 MW of installed electric capacity [3].

In addition to producing clean biofuels, AD has other advantages. This is, for example, solving the problem of waste disposal by burying. Thus, the use of AD technology helps reduce the unpleasant odor from the decomposition of waste and reduce greenhouse gas emissions.

It is important to note that the potential of biogas as a source of alternative energy makes AD the most cost-effective and environmentally friendly technology for waste treatment, compared to disposal, composting, and incineration. This is due to the fact that the production of energy from biogas has many advantages over other types of alternative energy. Firstly, it is the possibility of using a variety of organic materials: from energy crops and livestock waste to wastewater, which makes it possible to have regional raw materials for production and reduce the cost of its logistics [4]. Secondly, it is the relative simplicity of the technological designs of anaerobic digestion plants in comparison with the production of traditional fuels [5]. In addition, the production of renewable energy using AD is not affected by external weather conditions, which makes it suitable for stable continuous production of electrical and thermal energy.

However, AD technology also has drawbacks. Thus, biogas contains residues of microorganisms [6], other gases, such as hydrogen sulfide and ammonia nitrogen, which often need to be purified. However, digestate can immediately be used in agriculture due to its composition to improve soil characteristics.

The main disadvantage is the low efficiency of anaerobic digestion enterprises. This is due to the complexity of the biochemical fermentation process. This can explain the fact that the average use of capacities in terms of electricity production in general is much lower than the technically determined efficiency of 90–98 % [7]. In this case, the indicator varies for installations of different power. Thus, low-power installations reach high levels of power use up to 92 %, and large anaerobic digestion plants operate with fairly low coefficients at the level of 60 % to 70 %. This clearly indicates the need to optimize the operation of installations since up to 40 % of the plant's capacity remains unused.

Given the current situation in the global energy sector and the advantages of the method, we can say that the study of the potential of biogas is an extremely relevant issue.

2. Literature review and problem statement

One of the most promising methods for predicting biogas yield is the use of mathematical modeling. There are many theoretical models describing anaerobic digestion systems by determining their biochemical, biological, and physicochemical processes.

The most common modeling method is the construction of an anaerobic digestion model ADM1, developed by IWA Task Group for «Mathematical modeling of anaerobic digestion processes» [8]. This model was built to simulate the process of anaerobic digestion of sewage sludge. ADM1 describes the most important stages of the process from substrate degradation to biogas accumulation, using dynamic balances, kinetics, and acid-base equilibrium equations. The model takes into account reactions such as the decomposition of organic acids, ammonia, and bicarbonate, as well as the release of methane and carbon dioxide. The ADM1 model is universal and can be customized for specific processes.

In a number of studies, this method is used as an optimization tool. Thus, in study [9], ADM1 was applied to determine the optimal speed and time of hydraulic retention to increase the rate of biogas production.

However, ADM1-based models can only be used with available experimental data under predetermined conditions and cannot be used to predict process performance under unexplored operating conditions.

In general, methods of mathematical modeling of biogas yield processes can be classified into several groups. These are methods that are based on time series; methods based on deterministic factor and stochastic correlation dependences; methods of statistical theory of learning [10].

These methods have one significant drawback: the uncertainty of results. The presented models are never certain, especially with a shortage of input data, which can be observed in studies of the process of anaerobic digestion at large factories.

The most accurate are the methods of statistical theory of learning. These models first launch input and output data, then they are able to identify their relationships, can find a relationship between them (the so-called learning process) [10]. Models do not require a large number of experiment or measurement attempts; they obtain data by comparing an existing database. This is an important point for experiments such as the study of biogas yield during anaerobic digestion. The fact is that when it is carried out it is difficult to create the same conditions, especially when it comes to significant time intervals. At the same time, the presented methods have a high ability to simulate changes in time. The most common in this group are the methods of artificial neural network and the method of the system of adaptive neuro-fuzzy inference [11].

These models have high accuracy, but they possess a number of disadvantages. In particular, this is the need for deep and long preparation, the presence of a local minimum, difficulties in determining the network architecture. However, weighing all the advantages and disadvantages of existing groups of forecasting methods, the methods of statistical learning theory are the best to use.

In studies of anaerobic digestion, the use of machine learning methods in general and, first of all, the method of artificial neural network (ANN) is common [12]. ANNs are information processing systems, a computer model of the «black box», derived from a simplified concept of the human brain, for example, the ability to learn, think, memorize, and solve problems [13].

There are quite a few studies using ANN in the field of anaerobic digestion. Various studies have used ANN to predict the fraction of methane, biogas volume, wastewater characteristics, gas yield, and optimal biogas production in various industrial areas: food industry [14], agro-industrial sector [15]. Thus, in study [14] attention is paid to modeling the formation of biogas from the substrate of organic waste from food plants with livestock waste. At the same time, the percentage of the substrate mixture, pH level, reaction period and reactor temperature were considered as input parameters for the model. In [15], an effective model of biogas production from a mixture of agricultural waste and livestock waste with their preliminary chemical treatment has been developed. In studies [14, 15], the goal was to build specific models using ANN with different testing and training coefficients, and to determine the optimal structure of the ANN time series model and the number of neurons in the hidden layer of the selected model. Nevertheless, studies [14, 15] are narrow-profile and are based on the use of a specific type of substrate. Therefore, they cannot be applied to anaerobic digestion of raw materials from household waste.

The closest are the studies of biogas yield in experimental laboratory reactors [16, 17] and on the existing anaerobic digestion plant [18], in which ANN models for methane yield were developed.

Thus, in [16], the ANN was used to determine the biogas yield from AD as a function of the temperature in the reactor, hydraulic retention time, the content of solid and organic fractions and the pH level. And study [17] highlights the development of an ANN model to determine the potential production of biogas, the rate of methane production and the composition of gas during AD as a function of pH, volatile fatty acids, and solid fractions. Studies analyze the process of anaerobic digestion in a structured manner. However, these studies [16, 17] were carried out in the laboratory and their results are not comparable with the results of biogas yield at large enterprises. Simulation of the anaerobic digestion plant is a complex and time-consuming process. It is practically impossible to fully reflect the entire process of the installation by performing research in the laboratory since the productivity of biogas yield varies significantly depending on the influential characteristics and operating conditions. Therefore, the results of these studies cannot be used to optimize technological processes in the installation of anaerobic digestion.

Of particular interest is study [18], which simulated and optimized the process of biogas production on the methane tank of the Russaifah biogas plant (Jordan Biogas Company) in Jordan. The analysis is extremely complete as the operational data on the plant are given for 177 days. The study considers the effect of the influence of installation parameters on methane production. The developed multilayer model of the ANN with two hidden layers was trained to simulate the work of the methane tank and predict methane production. However, of concern in the study is the high error of the model (0.87). Such an error value for ANN may be characteristic when analyzing samples from factories with different biogas production conditions (power, energy consumption, type of substrate on which they work, etc.). However, in the study, information was collected at one plant, and therefore the conditions for building a network model were the same. Therefore, an effective model should have an error of more than 0.9. Also, the model cannot be applied to the entire flow of solid household waste since the substrate in the study is food industry waste: waste from restaurants, fruit and vegetable markets, dairy industry. Study [18] is extremely valuable but narrow-profile and can be used to predict the yield of biogas from waste.

Our review of the literature [16–18] found that ANN is an effective tool for modeling and predicting the impact of various operating parameters on biogas production using AD under mesophilic or thermophilic conditions. After establishing the influence of parameters, biogas production can be improved by optimizing the parameters under favorable conditions of anaerobic digestion.

Summing up, it can be argued that existing studies of the biogas yield potential were carried out either in the laboratory or evaluated the operation of a specific anaerobic digestion unit. However, there is no comprehensive generalized complete study of building a biogas production model and optimizing process parameters. This allows us to talk about the presence of significant limiting factors in the research. The laboratory conditions of the experiment do not allow for taking into account the technological losses of biogas that occur at real installations. Consideration of the operation of only one methane tank unit can lead to subjective judgments about the entire anaerobic digestion process. Therefore, it is not expedient for building a biogas yield model but can only be a useful tool for optimizing the operation of a particular production.

It can be argued that it is expedient to conduct a study on the optimization of biogas production parameters, which would be based on the performance indicators of several operating anaerobic digestion plants. In addition, an important factor in finding the dependence of biogas production parameters is that it is necessary to select plants with different operating parameters and different capacities. However, it should be noted that the data for a wide range of operating conditions of the anaerobic digestion process are limited and the available data are not enough to perform an accurate forecast and optimization of the process.

This predetermines the task of our study – to increase the yield of biogas at AD enterprises as a promising direction for energy production. There is an urgent need to optimize the efficiency of the anaerobic digestion process at high-power enterprises.

3. The aim and objectives of the study

The aim of this study is to optimize the efficiency of biogas production at anaerobic digestion enterprises with a capacity of more than 5 tons/day. This will make it possible to increase the efficiency of the anaerobic digestion process by optimizing operational parameters.

To accomplish the aim, the following tasks have been set:

– to select parameters for modeling the process of anaerobic digestion based on ANN, which affect the production of biogas and methane at anaerobic digestion plants operating on waste;

– to build and test the effectiveness of the developed model of the ANN-based anaerobic digestion process using several test data randomly selected from the experimental field;

– to offer optimal operational parameters of the plant operation at anaerobic digestion enterprises with minimal loss of biogas potential using the ANN model.

4. The study materials and methods

The object of our research is the operational parameters of the installation, which is used for anaerobic digestion.

The working hypothesis of the study assumes the possibility of optimizing the operational parameters of the anaerobic digestion process by modeling the workflow through the use of ANN to increase the productivity of biogas production.

The study is focused on optimizing the anaerobic digestion process at biogas plants. The substrate is household waste.

The study used data from existing anaerobic digestion plants to model the biogas production process and build a mathematical model. Information on the work of 7 anaerobic digestion enterprises, which use household waste as raw materials, is analyzed. The enterprises are located in one geographical region within Germany. Their same location and the same type of raw material substrate on which they work confirm the reliability of the information, its relevance, and suitability for solving the tasks of our study.

Optimization of the biogas plant is to optimize the parameters in order to fully use its potential for biogas production and reduce the cost of its production. Controlled factors for modeling the biogas production process are the operational parameters of the process.

The complexity of the AD process necessitates a detailed consideration of the operational parameters in order to control the stability of the process.

The main problems of the anaerobic digestion process are that methanogenic microorganisms are very sensitive to environmental changes. A sudden change in pH, temperature, or an increase in the content of organic matter or a change in the concentration of the substrate can lead to an imbalance in the fermentation process, which will cause the failure of the reactor [19].

Therefore, the selection of the most suitable factors representing the behavior of the monitoring process is a very important point for accurate modeling for the anaerobic digestion system.

The most important parameters that affect the production of biogas are the content of free volatile fatty acids, the total amount of solids, the composition of biogas, the yield of biogas, pH, temperature, etc.

The study involved the construction of an artificial neural network to simulate the working process of biogas production.

The operational parameters of anaerobic digestion plants were obtained from analytical reports.

The data were subjected to a screening process to decide which among the known are the most consistent and correlated operating parameters, for their use in the development of the ANN model.

The ANN models are implemented using the Neural Network Tool of the Matlab 2014a software package.

Using the tool, 12 neural networks were built. The difference between the constructed models was the use of different learning functions: the Levenberg-Marquardt method («trainlm» function), Bayesian regularization («trainbr» function), gradient descent («traingd» function). To select a model, the step of the number of neurons in the hidden layer changed: 5–6–8–10.

According to the error criteria, a model with the highest generalizing ability was selected and, on its basis, the optimal performance indicators of the plant were selected, according to which the highest volume of biogas yield is expected.

Based on the developed ANN model, optimal operational parameters for the operation of installations at anaerobic digestion plants with minimal loss of biogas potential were selected.

5. Results of modeling and optimization of biogas production using an artificial neural network

5. 1. Selection of parameters for building a mathematical model based on an artificial neural network

5. 1. 1. Stating the optimization problem of the operating parameters of the anaerobic digestion installation process

To solve the task of optimizing the operation of the anaerobic digestion unit, the principle of its operation is described. To this end, the main input, output variables, as well as important factors of influence are determined (Fig. 1).

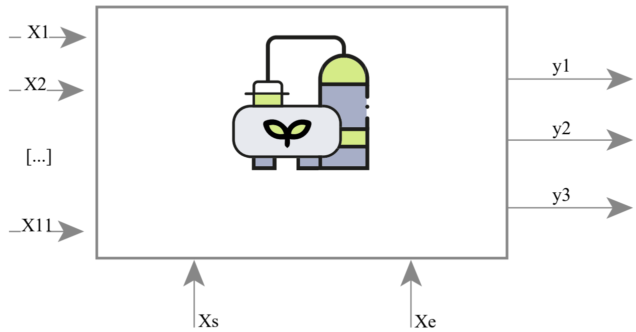

Fig. 1. Description of plant operation: optimization criteria: y_1 – biogas yield potential, y_2 – biogas volume, y_3 – potential loss of methane; controlled factors: x_1 – hydraulic retention time, x_2 – volumetric organic content, x_3 – reactor temperature, x_4 – pH value of the material, x_5 – total amount of solids in the input material, x_6 – percentage of organic matter in the input material, x_7 – the ratio of organic matter to dry fraction, x_8 – the content of total nitrogen in the starting material, x_9 – the content of ammonium nitrogen in the starting material, x_{10} – the percentage of nitrogen ammonium in total nitrogen, x_{11} – content of free volatile fatty acids in the starting material; uncontrollable factors: x_s – substrate input, x_E – plant power consumption

In the process of anaerobic digestion, the number of controlled variables is insignificant, which is an advantage for the stability of the installation process, but it is a difficult question to develop process optimization parameters.

The following criteria for optimization are selected: biogas yield potential and biogas volume, which should be maximized; potential level of methane loss, which should be minimized.

Descriptive statistics of variables for the model are given in Table 1.

Table 1

Descriptive statistics of model variables [20]

Parameter	Designation	Dimensionality	Data			
			Plants ($N=7$)			
			Mean	Min.	Median	Max.
Input variables (x_1–x_{11})						
Hydraulic retention time	x_1	day	175.00	70.00	128.00	445.00
Volume content of organic matter	x_2	kg·oTS/m^{3}*d^{-1}	1.60	0.30	1.60	2.70
Temperature in the reactor	x_3	°C	38.80	38.00	38.50	41.00
The pH value of the starting material	x_4	–	7.80	7.30	7.70	8.30
Total solids in the input material	x_5	%	4.20	2.50	4.30	5.30
The percentage of organic matter in the input material	x_6	%	2.80	1.60	2.70	4.10
The ratio of organic matter to the dry fraction	x_7	%	64.70	54.80	64.10	77.40
Content of total nitrogen in the starting material	x_8	g/kg	5.20	3.90	5.30	6.30
Ammonium nitrogen content in the raw material	x_9	g/kg	3.90	2.10	4.20	5.20
Percentage of ammonium nitrogen in total nitrogen	x_{10}	%	66.10	55.00	70.40	73.00
Content of free volatile fatty acids	x_{11}	mg/l	2360.00	20.00	1510.00	7910.00
Target variables (y_1 and y_3)						
Biogas output potential	y_1	%	69.40	54.00	71.20	78.70
Volume of biogas	y_2	m^3/t	171.00	26.40	104.00	584.00
Potential loss of methane	y_3	%	3.80	0.39	2.90	11.30

All these parameters have a strong influence on the course of the anaerobic digestion process, its stability, and economic acceptability. In addition, these parameters are closely interrelated with each other, as well as with the characteristics of the raw material substrate and the main process inhibitors. For example, both pH and temperature determine the concentration of NH_3 and H_2S [20].

5. 1. 2. Operational parameters of biogas production

The anaerobic digestion system includes 11 inputs that were evaluated using a t-test with a total probability of 5 % to verify their overall significance. Evaluation of the influence of factors shows that all individual input data, with the exception of hydraulic retention time, have a significant impact on the cumulative yield of the formed biogas and methane.

A graphical interpretation of the influence of controlled research factors using a distance matrix and Kohonen maps is shown in Fig. 2. The data for construction are the operational parameters of 7 operating enterprises of anaerobic digestion (Table 1).

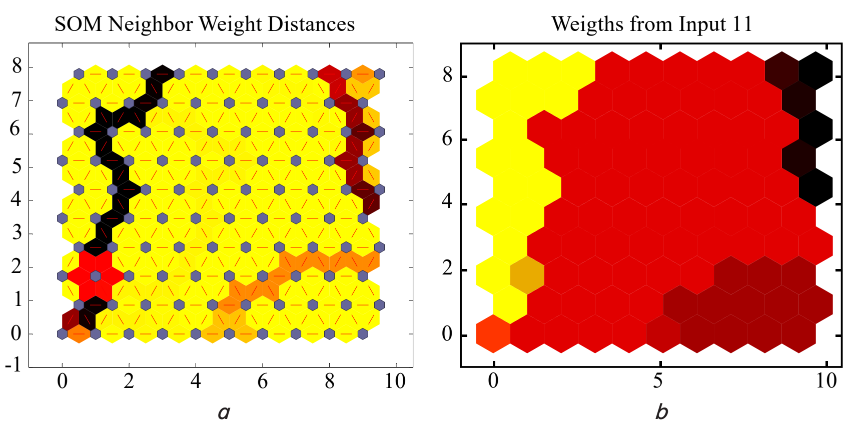

Fig. 2. Graphical representation of the influence of research factors: *a* — matrix of distances, size of 8×10 cells; *b* — Kohonen map, size 8×10 cells

The interdependence of factors is indicated by the same color of the honeycomb clusters of the diagram (Fig. 2).

In this case, the factor space is divided into 80 clusters, which is a rectangular table of 8×10 cells.

The most significant impact on the objective function of the model is exerted by the temperature in the reactor and the pH of the material, the hydraulic retention time, the volumetric content of organic matter. Also important are the following: the total amount of solids, the percentage of organic matter, the content of total nitrogen in the starting material, the content of free volatile fatty acids. These variables are adjusted to regulate in order to improve the quality and yield of biogas.

Below is a description of the main process parameters and operational parameters that are important for evaluating forecasting.

Hydraulic retention time (HRT). Methanogens double in 2–4 days, so a low HRT value may have a risk of leaching biomass from the reactor, which affects the stability of the entire process [21, 22]. If the retention time is less than 20 days, the substrate will not be able to be completely digested, which leads to a loss of energy. Thus, it is important to supply such an amount of substrate and with the appropriate intensity, to guarantee a retention time of more than 20 days.

Volumetric content of organic matter (OLR). The indicator has a strong impact on technological equipment, in particular on the design of circulation and feed pumps. High solids can increase pump wear. A low level of OLR is a factor in reducing the efficiency of biogas production. Nevertheless, the high OLR in the reactor is negative: it indicates the formation of inhibitory compounds, an imbalance of nutrients, and the accumulation of acid. Most anaerobic digestion plants operate with OLR in the range of 4.4–22 VS/l/day [23].

Reactor temperature. Temperature is one of the most important variables for the stability of the process. The fact is that populations of anaerobic bacteria can survive only in temperature ranges: from 20 °C to a maximum temperature of 60 °C. Temperature has an effect on the thermodynamic equilibrium of biochemical reactions and the diversity of microorganisms. The stability and speed of the process depend on it and, ultimately, it affects the yield of methane [24].

The process temperature must remain constant at any time to maintain stable operation of the installation. There are three different temperature ranges: psychrophilic – $T<25$ °C, mesophilic – 30 °C$<T<$45 °C, thermophilic – $T>50$ °C. Temperature increase affects all physicochemical mechanisms of the process: faster hydrolysis, less foaming in the reactor, reduced viscosity of effluents. Our study evaluated the work of enterprises operating in temperatures of both the mesophilic and thermophilic ranges.

The pH value. The pH is a key parameter of the process. It indicates the stability of the system. Methanogens are extremely sensitive to low pH; on the contrary, a high pH can lead to the formation of a toxic agent (free ammonia) [22]. The optimal pH value of the stable process is determined in the range from 6 to 9. The pH = 6 level indicates the process of inhibition due to high concentrations of volatile fatty acids, and a pH of more than 9 leads to a significant increase in ammonia, which also has a strong inhibitory effect.

Total nitrogen content and ammonium nitrogen content. The optimal concentration of nitrogen and nitrogen ammonium and their ratio inside the methane tank-reactor plays a crucial role in the stability of the anaerobic digestion process since it is a source of nutrients for microorganisms.

It is recognized [25] that concentrations below 20.0 g/l are optimal for anaerobic digestion. However, if its concentration drops below 1.40 g/l, the process is inhibited. Therefore, the optimal values of ammonia concentration can be data within the reference range from 1.40 to 20.0 g/l [26].

Content of free volatile fatty acids in the source material (VFA). The concentration of free volatile fatty acids provides important information about the efficiency and stability of the process. It is determined that concentrations below 1000 mg/l are stable for household waste [27], but not more than 20000 mg/l [27]. So, the reference limits accepted will be values from 1000 to 20000 mg/l.

5. 2. Development of a mathematical model of biogas production based on an artificial neural network

Since the polynomial approach to evaluate the effects of variables is not the most accurate for such complex systems as anaerobic fermentation, it was decided to apply a comprehensive study of the numerical model. Of all the existing methods of mathematical forecasting, a comprehensive assessment of several target variables can be performed only by constructing an ANN. After checking the impact of all variables, the practical implementation and training of the developed artificial neural network is made by means of the Matlab system, using the Neural Network Toolbox module.

The data were divided into the input matrix [x] and the target matrix [t]. A total of 11 variables related to the technological process were considered, among which, in particular, x_1–x_{11} (Table 1) were selected as input data of the ANN model [x], and the potential for biogas and methane production was taken as initial data [y]. The volume of biogas, the potential for biogas yield, and the loss of methane potential were determined as the initial target variables.

In the first step, each dataset was uploaded to the Matlab software workspace. The output network inputs and targets specified in the matrices [x] and [y] were normalized using the algorithm code, prestd.

The network was implemented and modeled using a learning feature based on the Levenberg-Markard optimization for reverse propagation training, as it showed the most satisfactory results in forecasting.

The sigmoid activation function is used as the basis since it is the most popular function that describes nonlinear dependences, such as biogas production. In addition, it was the sigmoid activation function that was able to simulate the operation of the methane tank reactor with high accuracy.

In this study, the ANN model for predicting biogas yield is based on:

– 3 levels: 11 input layers; one hidden layer with 8 neurons; three output layers of target variables. That is, a network of type 11–2–3 has been formed;

– type of network architecture: reverse propagation neural network;

– number of neurons in the hidden layer: from 5 to 10;

– type of activation functions: sigmoid function for layers of hidden level, linear for layers of the initial level;

– number of nodes in the input layer: 11 (Table 1);

– number of nodes in the output layer: 3;

– type of network error: RMS error and coefficient of determination.

A graphical representation of the proposed ANN modeling scheme is shown in Fig. 3.

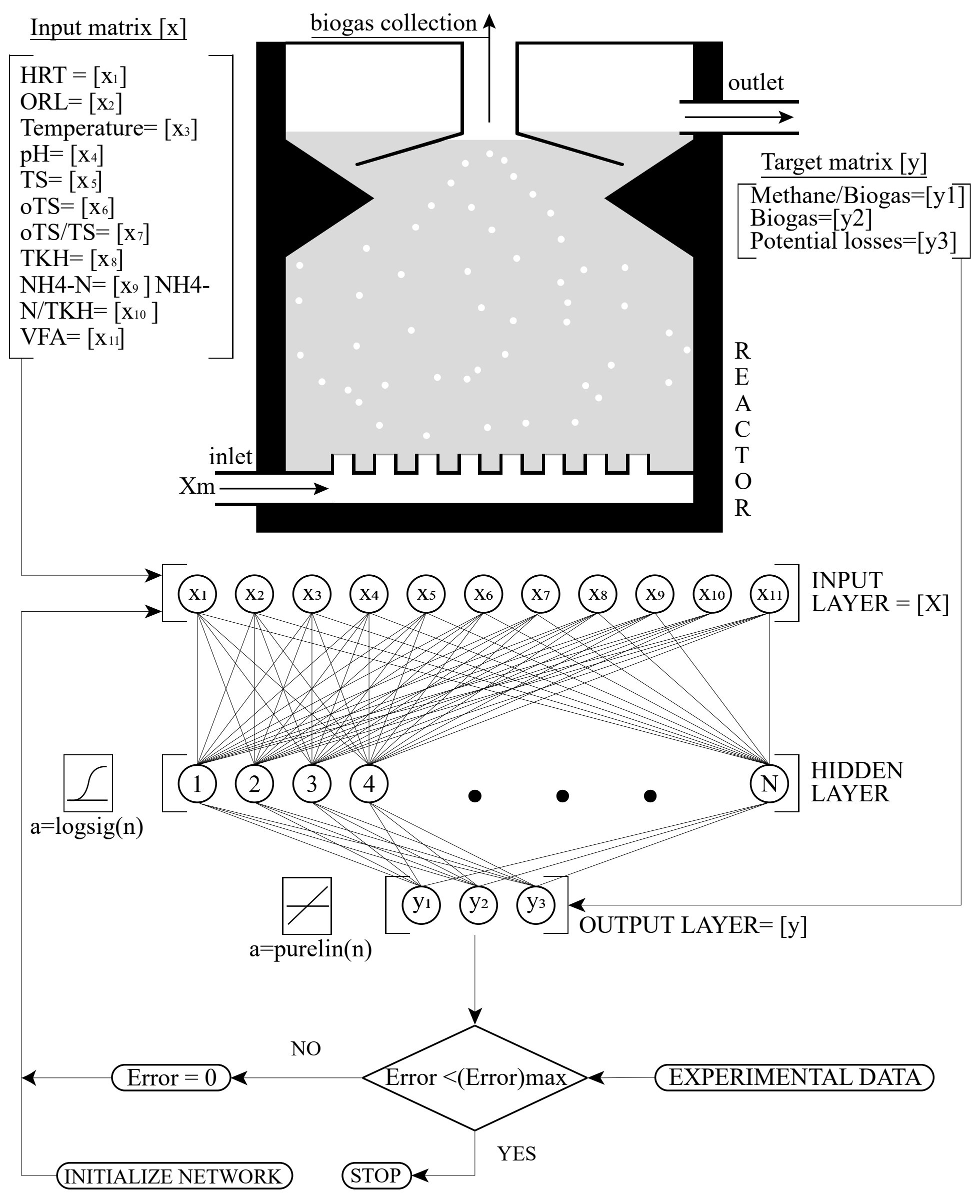

Fig. 3. Graphic diagram of the proposed model of an artificial neural network

To build a forecasting model at the first stage of building an ANNM, our data were divided into three parts: data for training, for validation, and verification. The training sample, respectively, is 70 % of the collected data, the samples for validation and verification are 15 % and 15 %, respectively.

To get the best model that simulates the work of a methane tank with minimal errors, several models of ANN were built and tested.

To select the optimal structure of the best ANN model, a different number of neurons in the hidden layer have been changed. The number of ranges that were analyzed ranged from 5 to 10. The optimally selected number of neurons in the hidden layer was 8.

In order to avoid overspending, the so-called retrainerability of the model, we used the early stop technique. More than 30 tests were conducted with randomly assigned inputs from the dataset to study the accuracy of the model and determine the case with a minimum MSE value. To assess the adequacy of the developed model, the coefficient of determination (R^2) and the standard error (*MSE)* should be considered. The result of modeling the selected models is given in Table 2.

For further evaluation, the optimal ANN model with the lowest MSE value at the testing stage was selected.

The Levenberg-Marquardt reverse propagation algorithm produced the best predictions for a training dataset in which R^2 ranged from 0.99 to 1.00. However, in application to the test dataset, performance declined slightly (0.89–0.99).

The Bayesian regularization algorithm showed significantly worse R^2 results than the reverse propagation algorithm and had a value of less than 0.10 at the validation and testing stage.

As for the test dataset, with R^2 in the 0.99 range, however, during the testing phase, the R^2 reached 0.00.

The gradient descent algorithm showed data values that vary significantly: in the range from 0.6510 to 0.9926 at the training stage; from 0.7267 to 0.999 at the validation stage, and from 0.0663 to 0.9964 during the testing phase, respectively.

In addition, it can be observed that in all cases the total number of parameters evaluated is always much lower than the total amount of data present in the database, which indicates a sufficient number of inputs and neurons in the hidden layer.

For all three learning algorithms, the stop criteria were reliable enough, so the models were not overtrained.

The architectural structure of the developed neural network for predicting the biogas yield is shown in Fig. 4.

Hidden Layer is a layer to the input of which signals are given, after which they are multiplied by weights (each signal is multiplied by its own weight) (in Fig. 4, indicated by the letter W). To this sum, one adds the displacement of the neuron (in Fig. 4, indicated by the letter b), and then enters into the summation block. The summation block algebraically adds weighted input data, creating an output. The resulting signal is transformed by the activation function of the neuron, which forms the output signal.

Determining forecasting patterns for 11 input signals and two hidden layers is a relatively difficult task. In this study, the number of iterations of learning was in the range from 9 to 9,751. Training ended when there was no noticeable improvement in results after a large number of iterations (8000 or more). Then we began checking the network for test data. As a result, only a few networks from a variety of trained ones turned out to be suitable.

The graph of the general distribution of data of the modified neural network at the stages of training, testing, and validation is shown in Fig. 5, *a–c*; graph of the whole model – Fig. 5, *d*.

The target *T* is the experimental cumulative volume of biogas and methane, while the yield *Y* is the ANN prediction of the target *T*. Linear correspondence is a linear regression between the initial indicator *Y* and the target *T*, and its ideal shape will be $Y = T$.

The above graphs (Fig. 5, *a–c*) of regression reflect the ratio of network outputs to target values for the training, verification, and test sequence.

Table 2

The resulting performance of the developed models

Model number	Neuron qty	*MSE*/R^2	Stages			Number of iterations
			Training	Validation	Testing	
Levenberg-Marquardt algorithm						
1	5	*MSE*	$3.90e^{-25}$	$1.41e^{-24}$	$595.74794e^{-5}$	4 000
		R^2	0.9999	1.0000	0.990559	
2	6	*MSE*	5.58659e-26	4.37975e-27	178.78685e-7	5 000
		R^2	1.0000	1.0000	0.89535	
3	**8**	*MSE*	$\mathbf{1.44012e^{-19}}$	$\mathbf{5.44340e^{-22}}$	$\mathbf{3.72e^{-14}}$	**8 000**
		R^2	**1.00000**	**0.99999**	**0.994696**	
4	10	*MSE*	2.02007e-27	4.38E-27	78.08065e-19	9 751
		R^2	0.9999	1.00000	0.98835	
5	5	*MSE*	2.20143	0.00000	0.879702	1 000
		R^2	0.99938	0.0503	0.99994	
Bayesian regularization algorithm						
6	6	*MSE*	1.88754	0.00000	2646.86896	275
		R^2	0.99968	0.1017	0.50322	
7	8	*MSE*	6.62752e-28	0.00000	292.56316	44
		R^2	0.9999	0.8541	0.99997	
8	10	*MSE*	2.25721	0.0000	0.890662	1 000
		R^2	0.99937	0.0000	0.99994	
Gradiet descent algorithm						
9	5	*MSE*	2874.91637	566.23157	52293.43	9
		R^2	0.65106	0.999981	0.0663281	
10	6	*MSE*	51.50655	329.24104	1483.38146	23
		R^2	0.99488	0.997293	0.535386	
11	8	*MSE*	5751.33599	2389.68136	6163.48597	9
		R^2	0.865894	0.726732	0.996456	
12	10	*MSE*	520.96013	564.91577	747.39473	10
		R^2	0.992586	0.921147	0.902444	

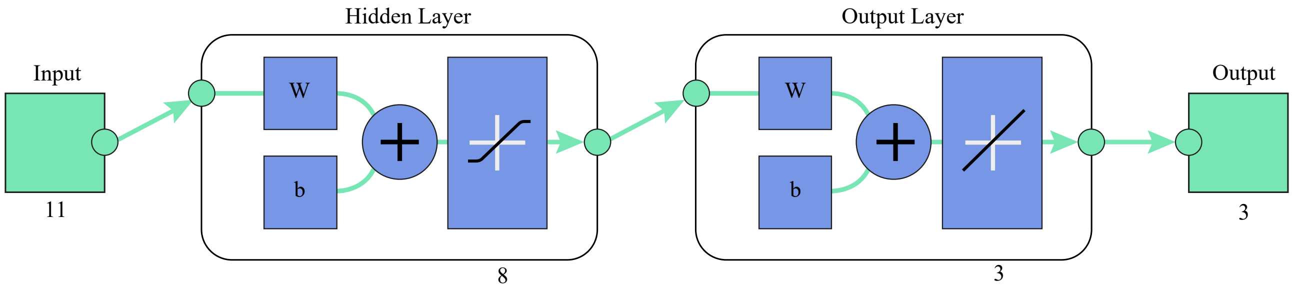

Fig. 4. Structural model of the proposed model of an artificial neural network for predicting the yield of biogas and methane

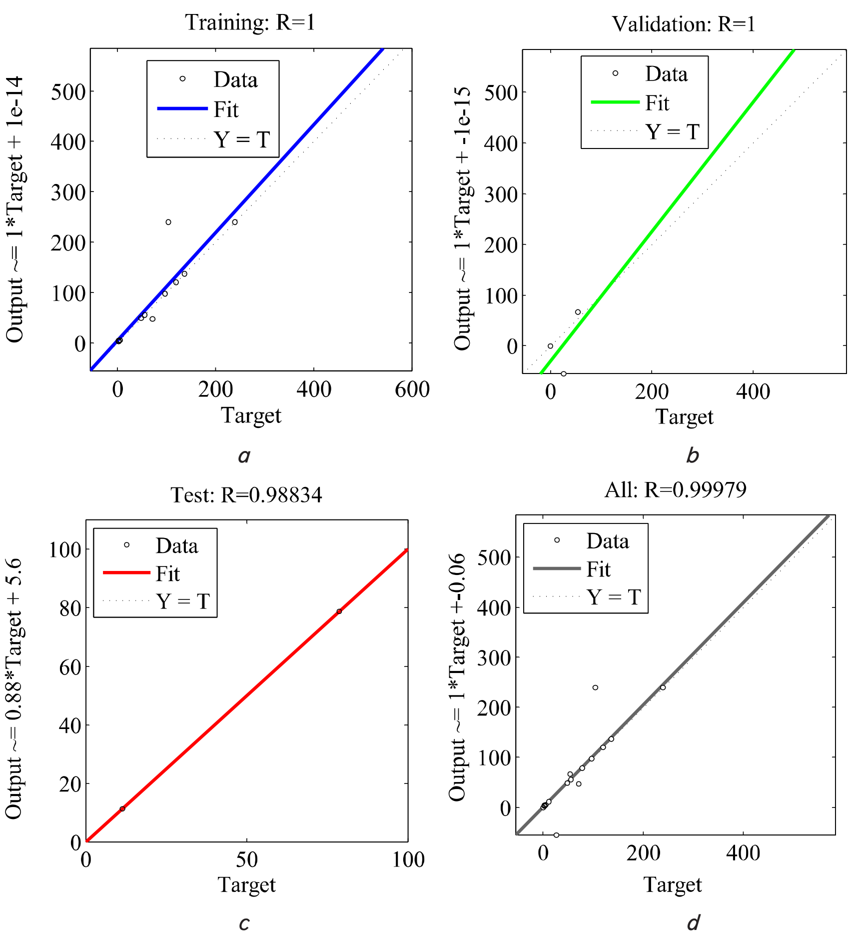

Fig. 5. Regression graphs at the stage:
a – training; *b* – testing; *c* – checking; *d* – general graph of the model

Along the abscissa and ordinate axes, the values of the final samples of the data of the trained neural network are arranged in the range from 0 to 600 at the training and testing stage and in the range from 0 to 100 at the validation stage. The reference values of vectors are displayed in the form of a dotted line, individual values of these corresponding parameters are marked with markers of the «circle» type, the line shows the correlation for all values of the model.

The developed model allows us, on the basis of a general analysis, to assess the effect of changing the values of input fuzzy variables on the values of output fuzzy variables.

The overall score (R^2) of the model is 0.99979, which indicates a very high accuracy and adequacy of the constructed model.

When optimizing the network as a conditional assumption, the selection began with two neurons in the hidden layer. With the increase in the number of neurons, several local minimum values and different MSE values were obtained for training sets in predicting the rate of biogas production.

The number of neurons in the hidden layer has been optimized as 8 with minimum mean values of MSE 4.3766e-27. When the number of neurons exceeded these global lows, MSE values increased significantly ($NH = 10$) for training datasets. This increase can be explained by the MSE performance index and the input vector characteristics [x] used in this study.

To check the model, we shall examine its convergence in individual areas in accordance with known data using network feedback. A graphical comparison of known values and estimated values of the neural network (during training and test sets) is shown in Fig. 6 and Table 3.

Table 3 shows that the largest error calculated in the ANN is 10 %; the smallest value of the ANN error is 3 %.

From MSE and the errors studied, it can be concluded that the proposed ANN is effective.

It can also be argued that the proposed model has a higher accuracy since it has smaller errors compared to the value of errors in the closest work of practical direction [18].

The obtained results show that the developed neural network has successfully mastered the basic dependence of biogas yield on input data.

During the test forecasting on the built neural network, a forecast was obtained with an error of not more than 10 %, which is a confirmation of the adequacy of the forecast.

The emergence of some disagreements that do not really correspond to the predicted values can usually be explained by a number of factors. This may be the result of inaccurate input data. Since the data were collected by different experts, it is possible to assume the presence of errors in experimental conclusions, the inaccuracy of instrumental data collection or observations. The neural network model will not give a coincidence between the actual and predicted values, unless the balances are really both negative and positive (Fig. 6).

The limitations for ANN are the values of the input parameters in which the process of anaerobic digestion takes place. They are as follows: hydraulic retention time: more than 20; volumetric content of organic matter: 4.4–22 kg·oTS/m^3; reactor temperature: 30–45 °C; pH value: 6–9. Also, the selection of parameters is limited by the content of total nitrogen in the starting material: 1.4–20 g/l; content of free volatile fatty acids in the starting material: 1000–20000 mg/l.

Table 3

Deviation of the data predicted by the model from known data

Indicator \ Atempt	1	2	3	4
Y_1 – the ratio of methane to biogas, %				
Known data	54.00	55.52	48.58	71.20
Model data	55.89	59.18	51.49	69.06
Absolute deviation	–1.89	–3.66	–2.91	2.14
Relative deviation	–3.50 %	–6.60 %	–6.00 %	3.00 %
Y_2 – biogas yield coefficient, Nm^3/t oTS				
Known data	126.40	136.80	119.70	104.00
Model data	134.78	135.14	122.58	106.07
Absolute deviation	–8.38	1.66	–2.88	–2.07
Relative deviation	–6.63 %	1.21 %	–2.41 %	–1.99 %
Y_3 – potential loss of biogas, %				
Known data	0.39	3.04	2.66	2.90
Model data	0.40	3.34	2.90	2.81
Absolute deviation	–0.01	–0.30	–0.24	0.09
Relative deviation	–3.70 %	–10.00 %	–9.20 %	3.00 %

Analyzing the known data and data of the ANN, it was found that the highest volume of biogas yield, determined by the simulation of the ANN, is 580.3 (m^3/t) at the temperature in the reactor of 41 °C, the pH value of 8.30, and the volumetric content of organic matter of 4.70 kg·oTS/m^3. Compared to related studies [18], this is the best indicator of the effectiveness of ANN.

During the learning procedure on known data, they are correlated using linear regression, trying to reach $R^2 = 1.00$ in learning value systems as shown in Fig. 5. It was found that regression can be compared with other works for both validation and testing, with regression being 0.99979 in the general case of the model, which is a higher result compared to related studies [18].

5. 3. Determination of the optimal parameters of the plant operation with minimal loss of biogas potential

Optimization of industrial processes, component design, and simulation models is often very complex and time-consuming, particularly if these optimization problems are highly scalable and nonlinear. The use of the developed ANN model made it possible to facilitate the selection of optimization parameters of the anaerobic digestion unit to increase the level of biogas production.

Optimization was done using Matlab tools. Selected optimized parameters of the installation are given in Table 4.

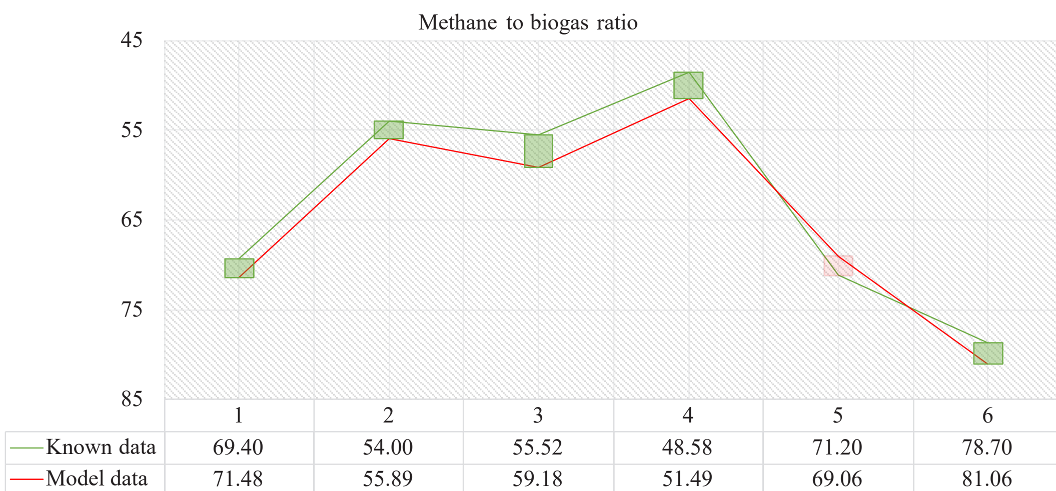

Fig. 6. Results of prediction of the performance of an artificial neural network in comparison with actual data

Table 4

Selected optimal parameters for the operation of the anaerobic digestion unit and their deviation from actual ones

Parameter	Designation	Value	Optimized parameters	Deviation	
				from min	from max
Input variables (x_1–x_{11})					
Hydraulic retention time	x_1	day	440.0	84.1 %	–1.1 %
Volume content of organic matter	x_2	kg·oTS/m^3*d^{-1}	4.7	90.0 %	10.0 %
Temperature in the reactor	x_3	°C	39.0	2.6 %	–5.1 %
The pH value of the starting material	x_4	–	8.0	8.8 %	–3.8 %
Total solids in the input material	x_5	%	4.5	44.4 %	–17.8 %
The percentage of organic matter in the input material	x_6	%	4.4	63.6 %	6.8 %
The ratio of organic matter to the dry fraction	x_7	%	97.8	44.0 %	20.8 %
Content of total nitrogen in the starting material	x_8	g/kg	6.5	40.0 %	3.1 %
Ammonium nitrogen content in the raw material	x_9	g/kg	5.5	61.8 %	5.5 %
Percentage of ammonium nitrogen in total nitrogen	x_{10}	%	84.6	35.0 %	13.7 %
The content of free volatile fatty acids in the raw material	x_{11}	mg/l	5 410.0	99.6 %	–46.2 %

According to the model, the selected optimal operating parameters of the methane tank reactor can increase the biogas yield by more than 12.6 %. The optimal indicators are: temperature, 39 °C; pH level, 8.0; the ratio of organic to dry fraction, 97.8 %; ammonium nitrogen content, 84.6 %; content of free volatile fatty acids, 5410.0 mg/l.

6. Discussion of the results of modeling and optimization of biogas production

The parameters for modeling the process at anaerobic digestion plants operating on waste are the total amount of solids, the percentage of organic matter, the content of total nitrogen in the starting material, the content of free volatile fatty acids, etc. (Fig. 1). These variables are adjusted to regulate in order to increase the volume of biogas production.

According to the results of the assessment of impacts using a matrix of distances and the construction of Kohonen maps (Fig. 2, *a, b*), the parameters that have the greatest weight per volume of biogas formation were obtained. They are the hydraulic retention time, the volumetric content of organic matter, the temperature in the reactor, and the pH value of the material.

To solve the problem of selecting the optimal operational parameters of the process of operation of the anaerobic digestion unit using the ANN model, the principle of its operation is described. The selection of the model that best simulates the work of a methane tank with minimal errors was carried out by creating and testing several models of ANN. The study conducted more than 30 tests with randomly assigned inputs from the dataset to study the accuracy of the model and determine the case with a minimum MSE value (Table 1).

The resulting model (Fig. 3) is based on the Levenberg-Marquardt reverse propagation algorithm since it demonstrated the most satisfactory results in forecasting (Table 2). It can be observed that the diagram of input and target indicators is close to the function $Y=X$, which indicates a fairly good modeling (Fig. 5).

Fig. 5 illustrates the developed model of biogas production and its verification, depending on the operational parameters of the operation of the methane tank plant. It can be noted that the ANN is able to predict the yield of biogas very accurately, which indicates a close relationship between the flow of methane tanks and the methane fraction in the biogas flow. There is a strong correlation between the data used in the validation process and the projected values of the methane fraction, which is shown in Fig. 5, *a–c*. The high value of the coefficient of determination of the general model (R^2) of 0.99 indicates that the simulated values of methane coincide with the measured values used for verification.

Evaluating the error value for all three datasets, we can assume that the model is able to accurately predict the produced volume of biogas and methane for the input factors considered since the total R^2 of the model approaches 1.

Testing with a different number of neurons in the hidden layer made it possible to clarify the optimal structure of the model with the slightest error.

To solve the specific case of the proposed nonlinear model, the selection of the number of neurons was carried out. A wider range of the number of neurons from 5 to 10 was chosen to determine the optimized structure of the model. When changing, the number of neurons in the hidden layer will change the original result since the weight of each neuron changes, and the result of the model will be changed.

So, according to the analysis of the errors obtained, the developed forecasting model is effective and optimal.

Unlike [8, 9], where mathematical modeling is used by determining biological and physical-chemical processes, the developed model can adequately simulate the AD process at large factories. This is especially important in the case of lack of input data and under unexplored operating conditions. This becomes possible thanks to the use of the method of an artificial neural network, which is able to generate new data by comparing an existing database.

In addition, the difference between the proposed model and the models reported in [16, 17] in which they are built by ANN on the data of a laboratory experiment is a deeper search for the dependence of parameters. The proposed model is based on data from real operating installations. At the same time, the selection was carried out focusing on various parameters and characteristics, which makes it possible to assess the relationships and influences of various parameters on the course of the anaerobic digestion process. This was the result of working with a larger database and made it possible to optimize the parameters.

According to the results of the simulation of the anaerobic digestion process, the optimal value of the operational parameters was found (Table 4).

According to the optimization of the operational parameters of the installation-methane tank, it will be possible to increase the potential for biogas yield by 12.6 % to 700 m^3/t. However, a negative phenomenon with such parameters of the plant operation will be an increase in the potential loss of methane up to 3 %. This means that the flammability of biogas will decrease. The logical question arises of assessing the energy potential of the produced biogas, which will be the topic of future research.

Selected with the help of the developed model, the optimal parameters of the anaerobic digestion process can solve the problem of increasing biogas production at enterprises with a capacity of more than 5 tons/day.

The main limitation of identifying input parameters to consider is a significant seasonality of temperature fluctuations. With such dynamic indicators, the accuracy of determining the projected biogas yield is significantly lost. Therefore, the condition for the use of the model is the stability of the specified optimal parameters. Failure to take into account the factors of temperature fluctuations can lead to the fact that the results obtained, even in the selected planning area, will not be entirely true.

Practical use of the proposed model of biogas production based on ANN is possible when monitoring work, increasing process efficiency, and adjusting the working conditions of the methane tank.

The study has certain limitations. The optimal parameters selected using the ANN model can be used only for enterprises of anaerobic digestion with direct heating. However, it cannot be used for enterprises with indirect heating, as it causes overheating and uneven heating of raw materials, and therefore the results of forecasting the biogas yield will be distorted. In addition, as a response function, only the operational parameters of the installation. But of scientific and practical interest are also the morphological composition of the substrate used for the production of biogas.

The disadvantage of the study is that this method requires a large amount of data from different sources. As a result, the data may be limited due to a contractor error or a malfunction of the measuring devices. One of the disadvantages of this method is that to improve the accuracy of the forecast, it is necessary to use a large amount of training data collected under similar conditions. However, in the case of AD enterprises, this is extremely problematic since there are a small number of those operating on the same substrate composition. It should be noted that seasonally, even at one enterprise, the composition of the substrate changes, which also affects the accuracy of the data.

In the future, it is planned to compare a simulation laboratory experiment with different types of substrate and compare its results with the data of working AD enterprises.

The development of the study will be to improve the database: more data should be included for better network learning. In the future, the neural network can be retrained by increasing the number of training samples to develop a more accurate assessment model.

It is planned that future research will be aimed at studying the effect of the composition of waste on operating parameters, as well as on the amount of biogas generated in the methane tank. For a certain type of biomass, more reliable models should also be obtained. Parameters that were not considered in this study (e.g., inoculate and nutrient characteristics), and which currently contribute to the uncertainty of predictions, can also be added to improve the model.

The results obtained in the study should be tested and tested on a full-scale operation of the plant in order to optimize methane production.

7. Conclusions

1. The operational parameters of the methane tank reactor at anaerobic digestion enterprises with a capacity of more than 5 tons/day have been estimated. They were chosen as input characteristics for the implementation of the ANN approach. It was found that the temperature and pH parameters have the greatest impact on the productivity of biogas and methane production. Also, important factors influencing the production of biogas are the total amount of solids in the input material, the percentage of organic matter in the input material, and the content of total nitrogen in the starting material. It is substantiated that ANN is a powerful data modeling tool that is capable of recording and representing complex input/output connections, as in the case of simulating the anaerobic digestion process to produce biogas.

2. A mathematical model based on an artificial neural network has been built to predict biogas production in biogas reactors with a capacity of more than 5 tons/day. It was found that the reverse propagation ANN model with two hidden layers and sigmoid activation functions captures most of the important patterns of biogas formation since it is well consistent with the measured biogas yield indicators at existing reactors. The error of the ANN model ($R^2 = 0.99$) indicates that the ANN is a useful tool for predicting biogas production in methane tank reactors of anaerobic digestion enterprises. Our study also demonstrated the importance of selecting the number of network neurons and algorithms to accurately describe the methane production process. To assess the performance of the model, the coefficient of determination (R^2) and the quadratic mean error (MSE) were used. Both approaches showed good results in forecasting and showed good consistency with experimental data. The model demonstrates high prediction accuracy with satisfactory MSE and R^2 at 37.16E-15 and 0.9996. This testifies to the effectiveness of the developed approach to predicting the yield of biogas and methane and can be an effective tool for coordinating the operating modes of anaerobic digestion plants and technical and economic studies.

3. The developed ANN model made it possible to identify the optimal operating parameters of the methane tank, which lead to an increase in methane yield by more than 12.6 %. Thus, the optimum temperature for increasing the biogas yield is 39 °C; pH level, 8.0; the ratio of organic matter to dry fraction should be 98.8 %. For better operation of the installation, it is necessary to increase the content of ammonium nitrogen by 5 % while the content of free volatile fatty acids in the substrate should be reduced by 46 %. The study demonstrated that the ANN model is a useful tool for modeling and optimizing biogas production from methane tanks under different operating conditions.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study and the results reported in this paper.

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Data availability

All data are available in the main text of the manuscript.

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