Modeling the Biogas Production Process in Biogas Plants Using Regression Analysis*

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Abstract

The problem of modeling the biogas production process in biogas plants based on regression analysis of data obtained from a specific biogas plant is considered. The influence of factors such as pH level and the composition of organic materials, taking into account specific time points and the volume of their addition to the fermentation medium (substrate), on the efficiency of this process is demonstrated.

The Lasso regression method (Least Absolute Shrinkage and Selection Operator) from the Python sklearn library was used to build the model.

It was established that changes in the operating parameters of the biogas plant can have a delayed effect, and based on this, the constructed regression model also considers the impact of previous values in the data sample in the form of the pH_lag2 parameter. To assess the accuracy of the obtained model, metrics such as R^2 and mean relative error were used. After applying the derived equation to the test dataset, the R^2 value reached 0.8889, and the mean relative error was 7.86%.

Keywords

Biogas plant; identification; mathematical model; nonlinear optimization; pH of the environment.

1. Introduction

The increase in greenhouse gas emissions, particularly carbon dioxide (CO_2) and methane (CH_4), is one of the main factors contributing to global warming [1-2]. This underscores the importance of finding and implementing renewable energy sources, among which biogas plays a significant role. Biogas is produced through the anaerobic decomposition of organic waste, such as agricultural residues, food waste, and livestock manure [3-7]. It primarily consists of methane and carbon dioxide, with minor amounts of water vapor and other gases, allowing for a significant reduction in harmful atmospheric emissions [8-10].

Biogas production is an effective method of organic waste management, as it converts waste into a renewable energy resource. Anaerobic digestion helps reduce methane emissions, which would otherwise be released from landfills, while simultaneously creating an energy source that can be used for electricity, heat, or biofuel production [11-12]. Estimates suggest that with proper policy regulation and the implementation of efficient technologies, the biogas industry could reduce global greenhouse gas emissions by 3.29 – 4.36 gigatons of CO_2 equivalent, accounting for 10% to 13% of total global emissions [13-14].

Despite its significant environmental potential, the use of biogas production technologies is associated with several challenges, such as maintaining the continuous operation of production processes and stabilizing technological parameters.

For biogas plants to operate efficiently, it is essential to monitor key indicators, including temperature, pH level, methane concentration, and the carbon-to-nitrogen ratio. Proper control of these parameters allows for the maximization of biogas yield and ensures the stability of the

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production cycle [15-17]. Therefore, the search for new methods to control these parameters, including software-based approaches, is crucial for the development of biogas energy systems. The implementation of such control requires the development of a mathematical model. In the theory of mathematical modeling, there are two main approaches: deductive and inductive [18]. In the deductive approach, the mathematical model is built based on physical principles [18]. This method requires adjusting the model for a specific type of biogas plant, and the model itself must incorporate physical parameters that need to be measured, which poses a challenge. In the inductive approach, the mathematical model is developed specifically for a given biogas plant, based on empirical data obtained from its operation [18-19]. This study adopts the inductive approach to model biogas production.

At the same time, in the inductive modeling approach, an important consideration is ensuring the accuracy of experimental results. When dealing with a limited dataset, interval data analysis is typically used for model construction [20-25]. However, if the dataset is sufficiently large, it is more appropriate to apply regression analysis [26]. Additionally, since structuring a regression model is inherently an intelligent process, it is beneficial to use a well-established software environment for this purpose. In our case, we chose Python libraries [27]. The choice of this environment was influenced by the availability of the Least Absolute Shrinkage and Selection Operator (Lasso) from the sklearn library. A key advantage of this method is its built-in regularization procedure, which helps prevent overfitting and enables automatic elimination of low-significance parameters.

2. Literature review

The authors of the work [28] investigate the stages of fermentation, taking into account biochemical processes, with the aim of ensuring the stability of biogas production. In [28], a new modified dynamic mathematical model is presented for simulating the biochemical and physico-chemical processes of biogas production during anaerobic fermentation. It should be noted that the proposed model includes data on the biochemical structure along with additional information about the physico-chemical processes of fermentation. In this work, the researchers confirmed the ability of the proposed mathematical model to generate accurate data on anaerobic fermentation processes using static indicators. The processes of anaerobic fermentation are discussed in works [29-31].

In works [32-35], models in the form of "black boxes" are investigated, which are built based on experimental data. These models can account for possible deviations at any stage of biogas production, and it is to this class that regression models belong, which are suitable for considering the type and structure of bioresources, as well as technological process parameters, including temperature, humidity, etc. Additionally, in work [35], a logistic equation is discussed for optimizing fermentation processes.

Although regression analysis is an effective method for identifying relationships, standard linear or polynomial regression does not always provide an accurate model, especially if there are nonlinear dependencies between variables. A serious issue with such models is overfitting, which occurs when the model memorizes the training data too well and identifies incorrect relationships. This negatively affects the accuracy of predictions for future data. To combat overfitting, a technique called regularization is used: by adding certain constraints to the loss function, a more flexible model can be obtained, preventing overfitting.Серед популярних методів, що включають регуляризацію, можна виділити Lasso-регресію та Ridge-регресію [36-37].

Both approaches aim to reduce the influence of coefficients on the final model. The main difference between them is that Lasso zeros out variables that have a weak influence on the prediction, while Ridge only reduces their values in the model. For this task, which involves predicting the volume of biogas produced based on dynamic substrate and acidity data, Lasso regression has proven to be more effective. The reason for this is that we need to eliminate values that create excessive noise when calculating the results. Specifically, this applies to the acidity values and their lags. Since we do not know at what moment and for how long the acidity influences the gas volume, we need to highlight only those values that had a significant effect on the prediction. According to the results, the strongest effect occurred after 2 days. All other variations only reduced the accuracy of the model and decreased its flexibility. Thus, Lasso regularization allowed us to remove redundant or insignificant coefficients from the final equation.

Separate approaches to solving regression tasks, based on the use of decision trees, include Random Forest and XGBoost. They also effectively find dependencies for dynamic data but do not allow for obtaining a mathematical equation. The result of their training is an ensemble of decisions, which is not suitable for this specific task. For the implementation of the regression described in this work, the scikit-learn (sklearn) library [38] was used. This is a popular Python library for machine learning. Its main advantages are ease of use, speed, and a wide range of algorithms for writing regression models. Additionally, Python is one of the most popular programming languages for machine learning, and its environment includes a large number of tools for solving related tasks. This allows for further improvements to the model, including combining different approaches to increase prediction accuracy. Moreover, Python tools allow for integrating this software solution into real projects, particularly by implementing an interface for working with the program on any platform.

3. Problem statement

The aim of this study is to develop a model for predicting the volume of biogas production in biogas plants based on regression analysis of data. Thus, the research task is to develop a mathematical model that would allow forecasting the output of biogas as a result of anaerobic microbiological fermentation in a biogas plant, depending on technological factors. As mentioned above, such technological factors include the pH level and the composition of organic materials, considering specific moments in time and the volumes of their addition to the fermentation medium (substrate). Based on this, it will become possible to optimize the operation of biogas plants, thus increasing the efficiency of biogas production.

In our case, for the development of a mathematical model for the pH of the environment in the biogas plant, the measurement results provided by LLC "Teofipil Energy Company" were used, in accordance with the project "Modeling the Dynamics of Processes in Biogas Plants," state registration number 0123U103785, commissioned by LLC "Zakhid Trade Ternopil," from September 12, 2023, to September 30, 2024, as well as the Ministry of Education and Science of Ukraine grant "Mathematical Tools and Software for the Prototype of a High-Efficiency Biogas Plant" (January 2024 – December 2025, state registration number 0124U000076), and the experimental data were obtained over 3 months – from May 1, 2024, to July 31, 2024.

A fragment of the measurement results is presented in Table 1. In the specified month, additional biomass was periodically loaded into the reactor for anaerobic fermentation.

Table 1
Results of experimental studies on the characteristics and parameters of the fermentation process

Date	pH	Gas volume	Substrate composition
01.05.2024	8,02	20800	s-0, p-107, m-20, c-5, st-260
02.05.2024	8,18	28380	s-0, p-122, m-17, c-5, st-317
03.05.2024	8,13	31600	s-0, p-80, m-14, c-5, st-274
04.05.2024	7,97	23293	s-0, p-58, m-10, c-6, st-300
05.05.2024	7,99	28908	s-0, p-87, m-14, c-6, st-280
06.05.2024	8,04	33518	s-0, p-77, m-17, c-6, st-300
07.05.2024	8,07	33347	s-0, p-71, m-10, c-6, st-310

It is also worth noting that these data include information about the date of biogas production and substrate loading, acidity (pH), substrate composition, and the volume of gas produced per day. It should be noted that changes in the operational parameters of the biogas plant can have a delayed effect, so the influence of previous indicators should also be considered when creating the model. The data on organic materials (substrate) contain information about the type and volume of each component: pulp (p), silage (s), manure (m), stillage (st), and chicken manure (c).

Thus, in this study, during the process of constructing a mathematical model of the pH environment in a biogas plant based on the analysis of interval data, the following tasks are addressed:

1) the selection of an appropriate regression analysis method, as well as the tools for its implementation using the Python library;
2) obtaining the structure of the regression model and identifying the model based on the use of the aforementioned library;
3) investigating the accuracy of the constructed regression model.

4. Method and results

4.1. Building a regression model

For modeling, the Lasso regression method (Least Absolute Shrinkage and Selection Operator) from the Python sklearn library was used. Its main advantages are the built-in regularization, which helps prevent overfitting of the model, and the automatic elimination of parameters that have a very low impact on the result. Through parameter tuning, the model was configured with a regularization parameter alpha = 0.01. To account for the delayed effect of changes in acidity, the parameter pH_lag2, representing a 2-day lag, was also added. Among various options, this value showed the best results when predicting the volume of biogas produced. In the future, as the number and values of the lag parameters increased, the model's accuracy decreased, indicating that the effect of acidity changes is highest after 2 days.

Before using the biogas production data for model training, they needed to be prepared and formatted. For this, a function was used.

```
prepare_data
def prepare_data(df, min_lag, max_lag):
  for material in materials_columns:
    df[material] = 0
  for index, row in df.iterrows():
    for material in materials_columns:
      match = re.search(rf'{material}-(\d+)', row['Materials'])
      if match:
        df.at[index, material] = int(match.group(1))
  for lag in range(min_lag, max_lag + 1):
    df[f'pH_lag{lag}'] = df['pH'].shift(lag)
  df['Date'] = pd.to_datetime(df['Date'])
  df['pH'] = df['pH'].astype(float)
  df['Gas'] = df['Gas'].astype(float)
  df.dropna(inplace=True)
  return df
```

To ensure correct results, data scaling was applied. Without scaling, features with larger values can dominate over features with smaller values, distorting the model's weight coefficients and its results. The StandardScaler method was used for scaling. The formula used by this method is as follows:

$$x_{scaled} = \frac{x - \mu}{\sigma} \quad (1)$$

where

μ – the mean value of the feature across the entire dataset

σ – the standard deviation of the feature

```
scaler_X = StandardScaler()
scaler_y = StandardScaler()
X_scaled = scaler_X.fit_transform(X)
y_scaled = scaler_y.fit_transform(y.values.reshape(-1, 1)).ravel()
```

After this, the scaled data were fed into the Lasso model, which in turn returned the coefficients for each of the parameters.

```
lasso = Lasso(alpha=0.01)
lasso.fit(X_scaled, y_scaled)
coefs = lasso.coef_
```

intercept = lasso.intercept_

As a result, the coefficients and parameters allow us to obtain the final regression equation.

final_coefs = [coef * scale_y / scaler_X.scale_[i] for i, coef in enumerate(coefs)]

final_intercept = mean_y + scale_y * (intercept - sum(coef * scaler_X.mean_[i] / scaler_X.scale_[i] for i, coef in enumerate(coefs) if coef != 0))

equation = f"Gas = {final_intercept:.4f}"

for feature, coef in zip(features, final_coefs):

  if coef != 0:

    equation += f" + {coef:.4f} * {feature}"

4.2. Final regression equation

The final regression equation obtained during the program's execution is as follows:

$$f(\vec{x}, y_{k-2}) = \beta_0 + \vec{\beta} \cdot \vec{x} + \beta_6 \cdot y_{k-2} \quad (2)$$

where $f(\vec{x}, y_{k-2})$ – the function that predicts the biogas volume (м³); $\vec{x} = (x_1, x_2, x_3, x_4, x_5)$ –the substrate mass vector (kg); x_1 – the mass of stillage; x_2 – the mass of pomace; x_3 – the mass of manure; x_4 – the mass of chicken manure; x_5 – the mass of silage; y_{k-2} – the pH value with a 2-day lag; $\beta_0 = -9551.4717$; $\vec{\beta} = (49.6650, 78.9349, 127.7447, 91.6091, 160.5516)$; $\beta_6 = 2051.2383$.

The coefficients of the variables determine their contribution to the prediction of biogas volume. The greatest influence is exerted by y_{k-2} (acidity two days later), which indicates the importance of historical acidity values of the environment. The contributions of silage and manure are also significant. At the same time, the acidity value on the same day was determined by the model as secondary and was excluded when constructing the corresponding equation.

To determine the accuracy of the obtained model, metrics such as R^2 and mean relative error were used. After applying the obtained equation to the test sample, R^2 showed a value of 0.8889, and the error was 7.86%.

Figure 1 shows the relationship between the predicted values of the produced biogas (Predicted gas amount) and the actual volume of biogas produced per day (Actual gas amount). The green area highlights the data that were used during the model training. It can be concluded that based on the obtained model, we can predict the volume of biogas produced for given input factors with sufficient accuracy. This is confirmed by the results of comparing the predicted gas volume with experimentally obtained values. However, there are still certain points where the obtained equation showed slightly inaccurate results. To ensure higher accuracy of the model, it is necessary to also consider other influencing factors in the construction of the model. Such factors may include temperature and humidity.

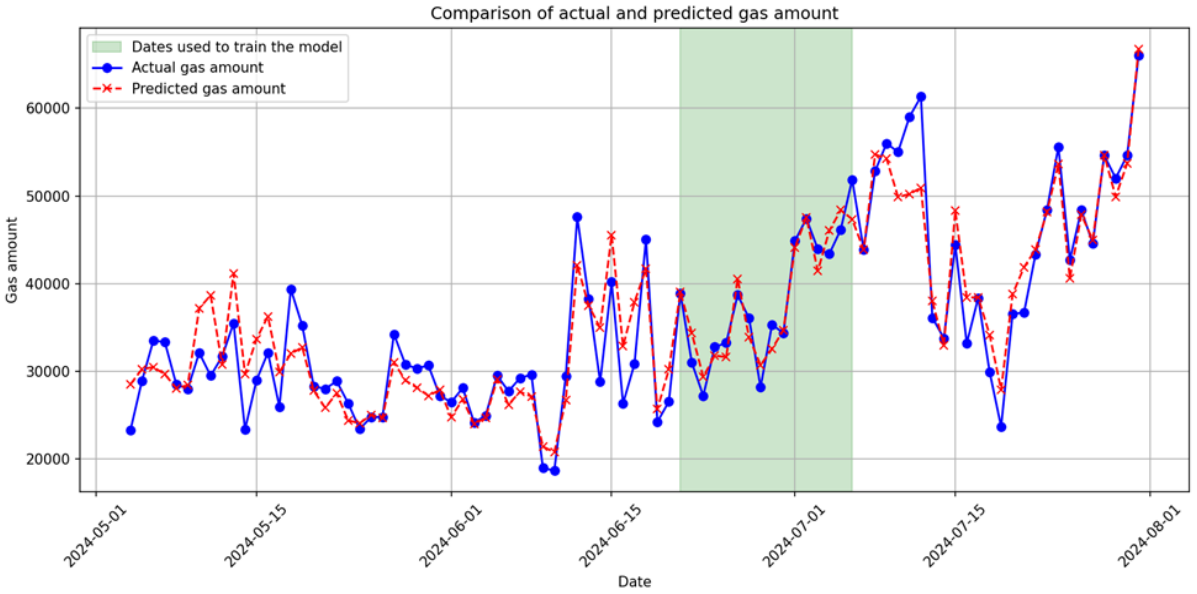

Figure 1: Results of comparing simulated values of biogas production and actual.

5. Conclusions

As a result of the conducted research, a mathematical model for predicting the volume of biogas production in biogas plants based on regression analysis was developed, which allowed for the consideration of technological parameters and time dependencies. For building the model, the use of the Python programming language was proposed and justified, specifically the sklearn library, which implements the Lasso regression method (Least Absolute Shrinkage and Selection Operator). The application of regularization in this method ensured the elimination of the "overfitting" effect and provided the simplest form of the model among the adequate models. Additionally, the model included a 2-day lag parameter, which accounts for the delayed effect of substrate acidity changes.

To determine the resulting accuracy of the model, metrics such as R^2 and mean relative error were used. After applying the obtained equation to the test sample, R^2 showed a value of 0.8889, and the error was 7.86%. Further development of the model may include expanding the data set, considering additional parameters such as temperature or humidity, and integrating with automated control systems for real-time monitoring. This will not only improve forecasting but also contribute to scaling up biogas technologies as an important element of green energy.

Declaration on Generative AI

The authors have not employed any Generative AI tools.

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