

A Simulation of Biogas Production from Lignocellulosic Biomass Co-Digested with Agricultural Waste under the Influence Bentonite Catalyst

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Abstract

This study aimed to simulate the effects of bentonite catalyst (B-cat) at different times into the digester containing maize cob, cow dung and food waste, using three different models. Data such as lag phase, maximum biogas production rate and cumulative biogas production were mined from an experiment, initially executed to determine whether difference in the application time of B-cat may cause any significant difference. Findings suggest that the data fitted well with both the modified Gompertz and Transference function models with R^2 in the range of 0.998 to 0.999 and fitting has been confirmed by the root mean squared error (RMSE) of 0.08 to 0.54, and 0.29 to 2.73 respectively for digesters where B-cat was applied at the onset of the experiment. For the dataset obtained when B-cat was applied one week after the commencement of the experiment, the RMSE was found in the range of 0.22 to 0.71 and 2.23 to 3.21 for MG and TF models respectively. The RMSE for LF model in both cases of times of application ranged from 0.54 to 4.86. Together, these suggest that the modified Gompertz and Transference function models have demonstrated the best fit with the experimental data compared with Logistic function model. In the design of digester for digesting maize cob with cow dung and food waste as co-substrates, the use of modified Gompertz and Transference function models are appropriate for the output estimation.

Keywords: Simulation, RMSE, Model, Maize Cob, Biogas.

Introduction

A model is an abstraction of reality and this abstraction represents a complex reality in the simplest way that is adequate for the modelling. The best model is always that which attains the greatest realism (measured objectively as agreement between model outputs and real-world observations, or less objectively as the process insight attained from the model) with the least parameter complexity and the least model complexity (Wainwright and Mulligan, 2002). Broadly, a model could be a scale model, a mathematical model, a sketch, a segment of computer code, an analogy, a working device, or many other things that can be used to describe or explain some aspect of the natural world. It can be used as part of the design of an artefact or an attempt to convince someone of some argument or ideology, or to determine public or corporate policy (Bissell and Dillon, 2012). Modelling and simulation is a tool that offers support for the planning, design, and appraisal of dynamic systems and the evaluation of strategies for system transformation and change. Its application

continued to grow at a notable rate because it is not limited by discipline borders (Birta and Arbez, 2013).

Lauwers *et al.* (2013) pointed out that there are two main approaches of model classification; dynamic or non-dynamic, and white-, grey- or black-box. Dynamic models use several ordinary differential equations. These models are fundamentally based on considerations of mass-balance to generate predictions continuous in time. Non-dynamic models link substrate to products, by means of stoichiometry through calculations of C, H, N and O and the gas yield to predict time-independent variables. White-box models are deductive and use prior information. Grey-box models are mechanistically inspired models including parameter estimation procedures while black-box models are data-driven models that link input directly to the output.

Mechanistically inspired anaerobic digestion models express the kinetics of stages of biogas production according to Monod-type kinetics, Haldane kinetics or Andrew kinetics. Most popular models of this group are Anaerobic Digestion Model no. 1 (ADM1), and parts of Benchmark Simulation Model no. 2. The Reduced Complexity Models express mass balance and process kinetics, and can be used for control strategies even for large-scale plants. Data-driven models, on the other hand, aimed at predicting the behaviour of the system without any pre-knowledge of the occurring process (Kucharska *et al.* 2018). Linear and non-linear regressions have been used previously in the simulation of cumulative biogas production (Li *et al.*, 2011).

Another classification put-forward by Lübken *et al.* (2010) showed that mathematical models of anaerobic digestion might be grouped into stoichiometry-based models, rate-limiting step models and multispecies models. Stoichiometry-based models assumed that biochemical composition decides the anaerobic digestibility of an organic substrate (Buswell formula & Boyle equation). The rate-limiting step approach highlights the need for the description of the rate-limiting step during the anaerobic digestions. The models apply Haldane kinetics, Andrew kinetics, Contois or Monod model. These are dynamic mathematical models which are like some mechanistically inspired models discussed by Lauwers *et al.* (2013). Multispecies models account for the complex microbiological consortia responsible for the anaerobic processes. An example of such model is again ADM1.

However, because of lack of universal classification of anaerobic digestion models, these authors (Kucharska *et al.* 2018; Lübken *et al.*, 2010; Lauwers *et al.*, 2013) have classified anaerobic digestion models into ADM1-based models, substrate conversion-based models, kinetic-based models, and black-box models. Veluchamy and Kalamdhad (2020) argued that kinetic model analysis is effective tool to control various anaerobic processes by providing suggestions related to reactor design and operation that may lead to a more efficient performance that reduces dependence on skilled operators and thus classified kinetic models into two major divisions as structural models and non-structural models.

A major limitation of structural models is their dependence on the metabolic pathways that are more complicated.

According to Adamu and Aluyor (2013), scientists researching on biogas production struggled to use several models to fit empirical data. Gibson *et al.* (1987) developed the MGM to a function that defines cell density during bacterial growth periods in terms of exponential growth rates and lag phase duration. This model was developed on the assumption that methane production rate in a batch digester corresponding to the specific growth rate of methanogenic bacteria (Kafle & Chen, 2016; Lay *et al.*, 1998).

Because the MGM is identified as a good empirical non-linear regression model and commonly used in the simulation of methane accumulation, Tsapekos *et al.* (2018) simulated experimental data obtained from digestion of biofibres subjected to mechanical pretreatment methods using the Modified Gompertz equation and found that more intense operation (Extreme pretreatment condition) was not associated with higher methane yield and a fair R^2 of 0.61 was obtained. They therefore recommended the application of non-structural models (Modified Gompertz, Logistic and Transference function models). Moreover, the use of only one model to simulate anaerobic process in an anaerobic reactor has been argued to be insufficient owing to its complexity. To sort this challenge, careful appraisal of different model outputs gives reliable and precise kinetic parameters and this brings the need for model comparison (Aromolaran & Sartaj, 2021).

Objective

The purpose of this paper is to simulate experimental data to identify which of the three models has the best fit with the experimental data.

Methodology

Source of Data

The data used in the simulation study obtained from a previously published work (Clarkson, 2023) carried out at the Federal Polytechnic Bali Taraba State. The data mined for use in the simulation include the lag phase, maximum biogas production rate, ultimate methane yield and cumulative biogas.

Models for the Simulation

The Modified Gompertz equation, Logistic and Transference Function models represented in equation 1, 2 and 3 were used in the simulation study. The simulation was run using the IBM SPSS Statistics 23 package and the results were analysed using the Microsoft Excel. All the models were re-written in a programme compatible with SPSS acceptable Language. Non-linear regression was chosen and parameters listed above were inputted. Data estimated for the models were plotted in Ms Excel.

$$B = B_0 \exp\left\{-\exp\left[\frac{R_{me}}{B_0}(\lambda - t) + 1\right]\right\} \quad . \quad . \quad . \quad (1)$$

$$B = B_o \left\{ 1 - \exp \left(- \frac{R_m \cdot (t - \lambda)}{B_o} \right) \right\} \quad (2)$$

$$B = \frac{B_o}{1 + \exp \left\{ \frac{4 \cdot R_m \cdot (\lambda - t)}{B_o} + 2 \right\}} \quad (3)$$

Where: R_m = maximum biogas production rate (ml/day), λ = lag phase (day), t = incubation time (day), $e = \exp(1) = 2.7183$, B is the cumulative biogas yield (ml), B_o is the ultimate biogas yield (ml).

Validation

The three models were validated and compared using the R^2 obtained from the results of simulation and the root mean squared error (RMSE) computed using equation 4.

$$RMSE = \sqrt{\frac{1}{m} \sum_{j=1}^m \left(\frac{d_j}{y_j} \right)^2} \quad (4)$$

Where: m represents the number of data pairs, y_j is the experimental biogas yield at j th value and d_j is deviation of experimental and predicted values.

Results and Discussion

Introduction of B-cat at the On-Set of Experiment

A set of experiments were conducted to determine the influence of introduction B-cat at different times on biogas production from maize cob co-digested with animal manure and food waste. The information in Figure 1 is simulation results of biogas production under the effect of 2.5 g B-cat introduced at the onset of the experiment.

Simulation using the modified Gompertz equation (MG) and transference function (TF) models have closely fitted well with the experimental data. The R^2 of 0.998 and 0.999 were respectively obtained for MG and TF models. The RMSE of 0.54 and 2.73 were found for MG and TF models. These values supported the inference earlier reported for these models. However, the logistic function (LF) model has an R^2 of 0.954 and RMSE of 4.16 suggesting that this model has poorly fitted with the dataset used in the simulation. Although, the R^2 and the RMSE computed for MG and TF models conflicted, R^2 is relative measure of fit while the RMSE is an index that measures the actual fitness of models to data. Therefore, MG model is the model with an output very close to experimental data.

The data in Figures 2 and 3 are the results of the biogas output from similar substrates composition under the effect of 3.5 g and 4.5 g B-cat. The results showed that all the models have taken similar paths as the experimental results except the LF model. The R^2 for MG and TF is 0.999 while that obtained using the LF model is 0.956. The computed RMSE of 0.08, 0.29 and 0.54 were obtained for MG, TF and LF models respectively.

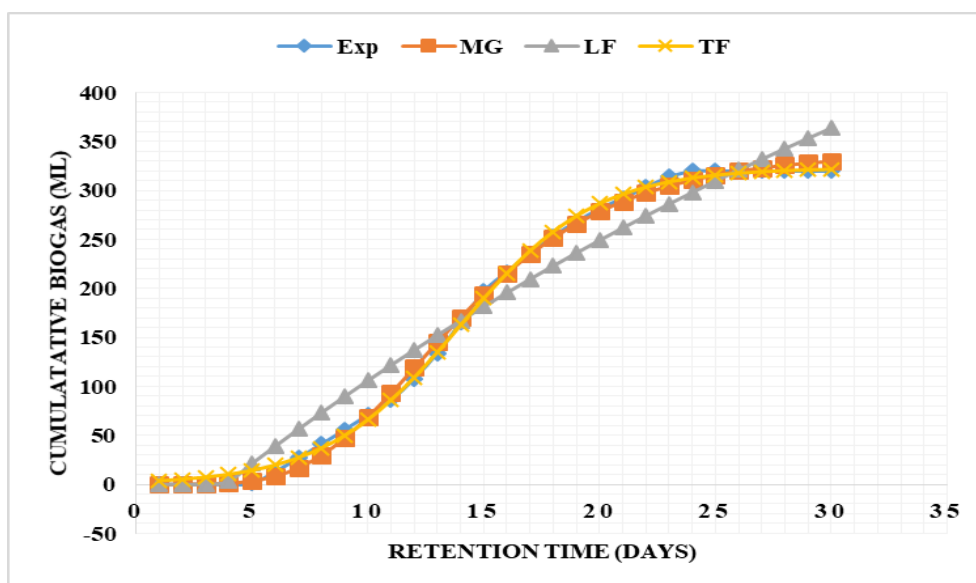


Figure 1. Results of simulation of biogas production under the influence 2.5 g B-cat applied at the on-set of the experiment.

The RMSE obtained when 4.5 g B-cat was introduced into the digester are 0.11, 0.72 and 0.35 for MG, TF and LF models respectively as shown in Table 1. The validation results for the dataset simulated using the three models all pointed that the LF model poorly fitted the data while MG model is the model with best fit having the lowest RMSE. The results of the present study supported the findings of Gidado and Clarkson (2022) where higher values of R^2 and lower values of RMSE were reported for MG and TF models.

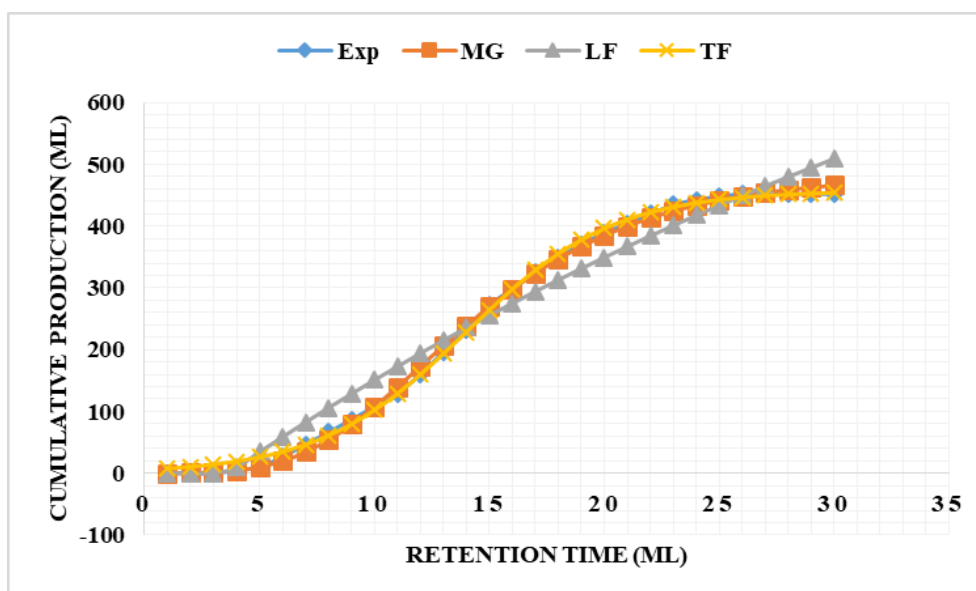


Figure 2. Results of simulation of biogas production under the influence 3.5 g B-cat applied at the on-set of the experiment.

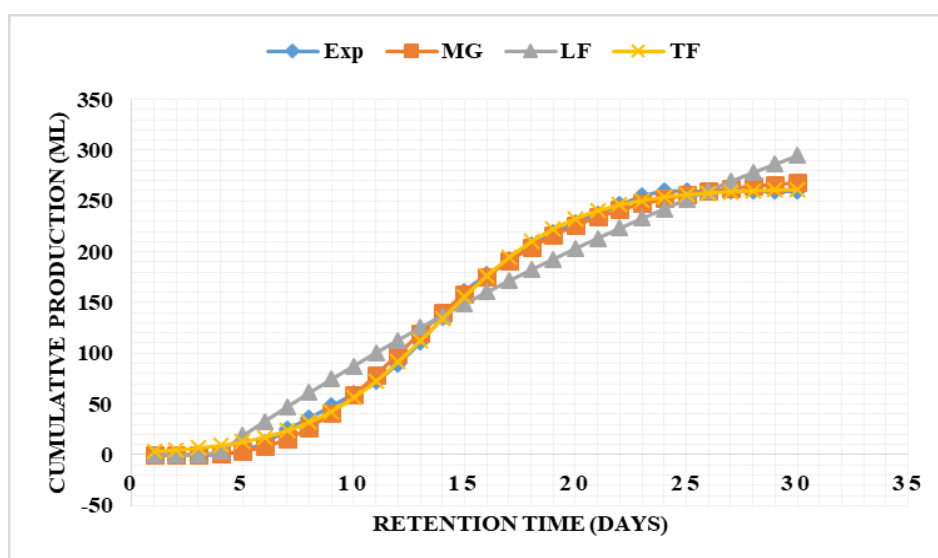


Figure 3. Results of simulation of biogas production under the influence 4.5 g B-cat applied at the on-set of the experiment.

Table 1. Root mean squared error for the models when the catalyst was applied at the on-set of the digestion.

Content of catalyst	Model		
	MG	LF	TF
2.5 g	0.54	4.16	2.73
3.5 g	0.08	0.54	0.29
4.5 g	0.11	0.72	0.35

Introduction of B-cat One Week into the Experiment

The B-cat was also introduced in the digester one week into the experiment and the results were simulated using the 3 models. The simulation results for the introduction of 2.5 g, 3.5 g and 4.5 g B-cat are shown in Figures 4, 5 and 6 respectively and the root squared mean error for MG, LF and TF models is also shown in Table 2.

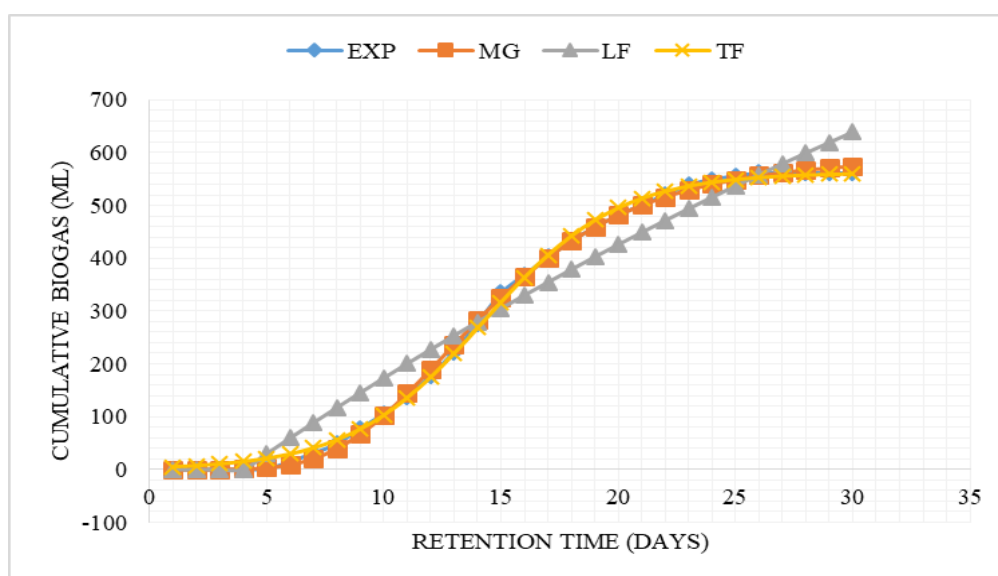


Figure 4. Results of simulation of biogas production under the influence 2.5 g B-cat applied one week after the beginning of the experiment.

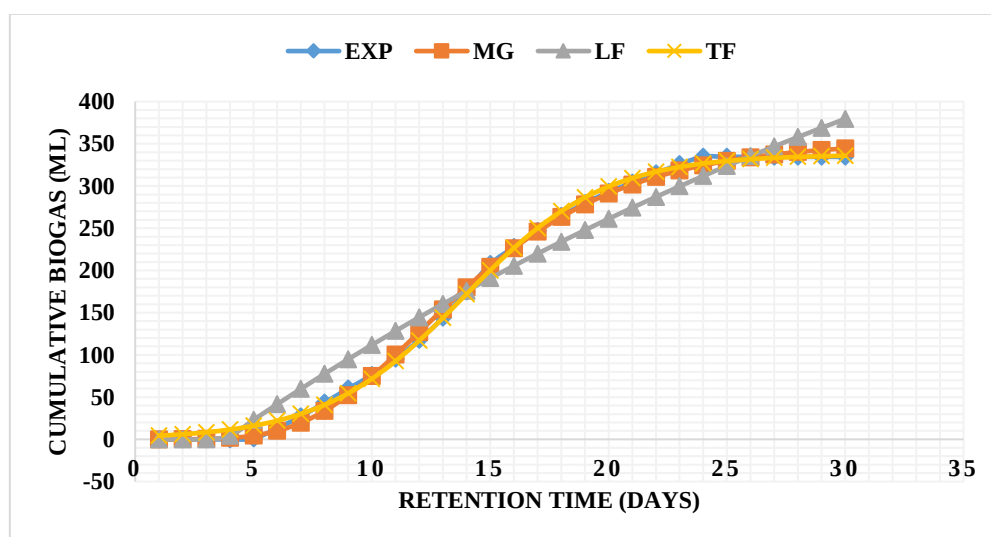


Figure 5. Results of simulation of biogas production under the influence 3.5 g B-cat applied one week after the beginning of the experiment.

The simulation results as graphically shown has shown a consistent pattern with the experimental data except the curve produced using the logistic function model predicting a straight-line relationship between the cumulative biogas production and the substrates retention time. This may further imply that there may be negative gas production which is practically impossible. The R^2 for the MG and TF models ranged between 0.998 and 0.999 while the RMSE for these models is in the range of 0.22 and 0.71 for MG model and 2.23 and 3.21 for TF model. However, the R^2 for LF model is well below 0.994 while the RMSE is in the range of 3.29 and 4.86. These indices suggest that logistic function model is a poor

estimator of biogas output form these substrates and for any simulation purpose or for design integration with digesters, the MG and TF models are better estimators. These findings have been supported by the results published by Li *et al.* (2012) where LF models performed well below that of the other models. The findings of this study are not consistent with the results reported previously (Elagroudy *et al.*, 2020; Musingarimi *et al.*, 2019).

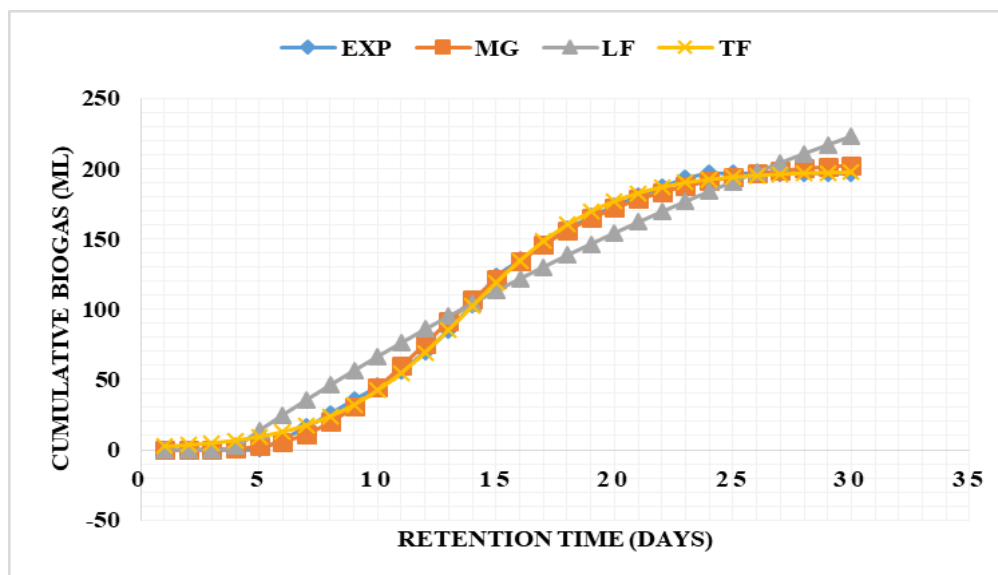


Figure 5. Results of simulation of biogas production under the influence 4.5 g B-cat applied one week after the beginning of the experiment.

Table 2. Root mean squared error for the models when the catalyst was applied at the onset of the digestion.

Content of catalyst	Model		
	MG	LF	TF
2.5 g	0.22	3.29	2.23
3.5 g	0.71	4.51	3.07
4.5 g	0.71	4.86	3.21

Conclusion

The main purpose of this article is to simulate experimental data obtained from co-digestion of maize cob, cow dung and food waste. It was found that the data fitted well with both the modified Gompertz and Transference function models with R^2 in the range of 0.998 to 0.999 and the fitting has been confirmed by the RMSE of 0.08 to 0.54, and 0.29 to 2.73 respectively for digesters where B-cat was applied at the onset of the experiment. For

the dataset obtained when B-cat was applied one week after the commencement of the experiment, the RMSE was found in the range of 0.22 to 0.71 and 2.23 to 3.21 for MG and TF models respectively. The RMSE for LF model in both cases of time of application ranged from 0.54 to 4.86. Together, these suggest that the modified Gompertz and Transference function models have demonstrated the best fit with the experimental data compared with Logistic function model.

Recommendations

1. In digester designs for purpose of digesting maize cob with cow dung and food waste as co-substrates, the use of modified Gompertz and Transference function models are appropriate for output estimation.
2. Further studies may try to investigate why Logistic function model failed to give close estimate of biogas production with contrasting patterns to that of experiment.

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References

- Adamu, A. A., & Aluyor, E. O. (2013). Empirical Model for Predicting Rate of Biogas Production. *Global Journal of Engineering Research*, 12, 63-68.
- Aromolaran, A., & Sartaj, M. (2021). Enhancing biogas production from municipal solid waste through recirculation of blended leachate in simulated bioreactor landfills. *Biomass Conversion and Biorefinery*, 1-16.
- Birta, L. G., & Arbez, G. (2013). *Modelling and simulation*. London: Springer.
- Bissell, C., & Dillon, C. (Eds.). (2012). *Ways of thinking, ways of seeing: Mathematical and other Modelling in Engineering and Technology* (Vol. 1). Springer Science & Business Media.
- Clarkson, M., A. (2023). Biogas Potentials of Maize Cob Co-Digested with Animal and Plant Waste under the Effect of Bentonite Catalyst. *Afropolitan Journals*, 12(1), 78-86.
- Elagroudy, S., Radwan, A. G., Banadda, N., Mostafa, N. G., Owusu, P. A., & Janajreh, I. (2020). Mathematical models comparison of biogas production from anaerobic digestion of microwave pretreated mixed sludge. *Renewable Energy*, 155, 1009-1020.
- Gibson, A. M., Bratchell, N., & Roberts, T. A. (1987). The effect of sodium chloride and temperature on the rate and extent of growth of *Clostridium botulinum* type A in pasteurized pork slurry. *Journal of Applied Bacteriology*, 62(6), 479-490.
- Gidado, M., & Clarkson, M. A. (2022). Modelling the Effects of Dilute Alkaline Pretreatment of Lignocellulosic Biomass on Biogas Production. *African Journal of Environmental Sciences and Renewable Energy*, 5(1), 49-57.
- Kafle, G. K., & Chen, L. (2016). Comparison on batch anaerobic digestion of five different livestock manures and prediction of biochemical methane potential (BMP) using different statistical models. *Waste management*, 48, 492-502.
- Kucharska, K., Hołowacz, I., Konopacka-Łyskawa, D., Rybarczyk, P., & Kamiński, M. (2018). Key issues in modeling and optimization of lignocellulosic biomass fermentative conversion to gaseous biofuels. *Renewable energy*, 129, 384-408.

- Kucharska, K., Hołowacz, I., Konopacka-Łyskawa, D., Rybarczyk, P., & Kamiński, M. (2018). Key issues in modeling and optimization of lignocellulosic biomass fermentative conversion to gaseous biofuels. *Renewable energy*, 129, 384-408.
- Lauwers, J., Appels, L., Thompson, I. P., Degreè, J., Van Impe, J. F., & Dewil, R. (2013). Mathematical modelling of anaerobic digestion of biomass and waste: Power and limitations. *Progress in Energy and Combustion Science*, 39(4), 383-402.
- Lay, J. J., Li, Y. Y., & Noike, T. (1998). Interaction between homoacetogens and methanogens in lake sediments. *Journal of fermentation and bioengineering*, 86(5), 467-471.
- Li, C., Champagne, P., & Anderson, B. C. (2011). Evaluating and modeling biogas production from municipal fat, oil, and grease and synthetic kitchen waste in anaerobic co-digestions. *Bioresource technology*, 102(20), 9471-9480.
- Li, L., Kong, X., Yang, F., Li, D., Yuan, Z., & Sun, Y. (2012). Biogas production potential and kinetics of microwave and conventional thermal pretreatment of grass. *Applied biochemistry and biotechnology*, 166, 1183-1191.
- Lübken, M., Gehring, T., & Wichern, M. (2010). Microbiological fermentation of lignocellulosic biomass: current state and prospects of mathematical modeling. *Applied microbiology and biotechnology*, 85(6), 1643-1652.
- Lübken, M., Gehring, T., & Wichern, M. (2010). Microbiological fermentation of lignocellulosic biomass: current state and prospects of mathematical modeling. *Applied microbiology and biotechnology*, 85(6), 1643-1652.
- Musingarimi, W., Okeleye, B. I., Okudoh, V. I., & Ntwampe, S. K. O. (2019). Prediction of biogas production from co-digestion of winery solid waste and zebra manure using modified gompertz model (GM) and logistic equation (LE).
- Tsapekos, P., Kougias, P. G., Alvarado-Morales, M., Kovalovszki, A., Corbière, M., & Angelidaki, I. (2018). Energy recovery from wastewater microalgae through anaerobic digestion process: Methane potential, continuous reactor operation and modelling aspects. *Biochemical engineering journal*, 139, 1-7.
- Veluchamy, C., & Kalamdhad, A. S. (2020). Effect of Total Solid Content of Lignocellulose Pulp and Paper Mill Sludge on Methane Production and Modeling. *Journal of Environmental Engineering*, 146(3), 04019121.
- Wainwright, J., & Mulligan, M. (2002). *Environmental modelling*. Wiley-Blackwell.