

A Study of Mathematical Models Used in Anaerobic Digestion of Organic Refuse

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Abstract The mathematical computation and process evaluation of anaerobic digestion (AD) treatment of organic refuse (OR) has become quite common in process designing. Furthermore, the modelling of AD process is considered as well-established and mature, and largely known as a mechanistic model structure. There are various mathematical models being used to comprehend the biochemical variations, rate of decomposition, and the methane or biogas production potentials. Moreover, these mathematical analyses of the models determine the computation of equilibrium points, helping to understand their internal stability with respect to feeding parameters, and compatibility to the output static characteristics of the entire AD process. Whereas numerical simulations are also carried out for specific biodegradation on web-based software. These simulations are useful to demonstrate the dynamic responses of the mathematical models to present the most mathematical viable solutions. However, the major issues lie in the application of AD in lab-based modelling needs improvement in characterization and the adaptation of new approaches to optimize bioenergy recoveries. Hence, this review paper discusses the selection and utilization of mathematical models for different conditions in AD treatment of OR for the best mathematical representations.

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1 Introduction

The exponential growth of population and urbanization have triggered the researchers to look and re-search for alternative sources of energy generation [1]. The harnessing of bioenergy (Be) from organic refuse (OR) through anaerobic digestion (AD) process is always considered as the most viable option. AD process is based on the four different stages as shown in Fig 1 and carried out in oxygen free environment [2]. It has been reported in literature that the AD process yielded positive result when any type of organic refuse or wastes such as agriculture, animal, crop residue, yard waste, food waste and sludge generated from the sedimentation of wastewater [3] as shown in the Fig 2.

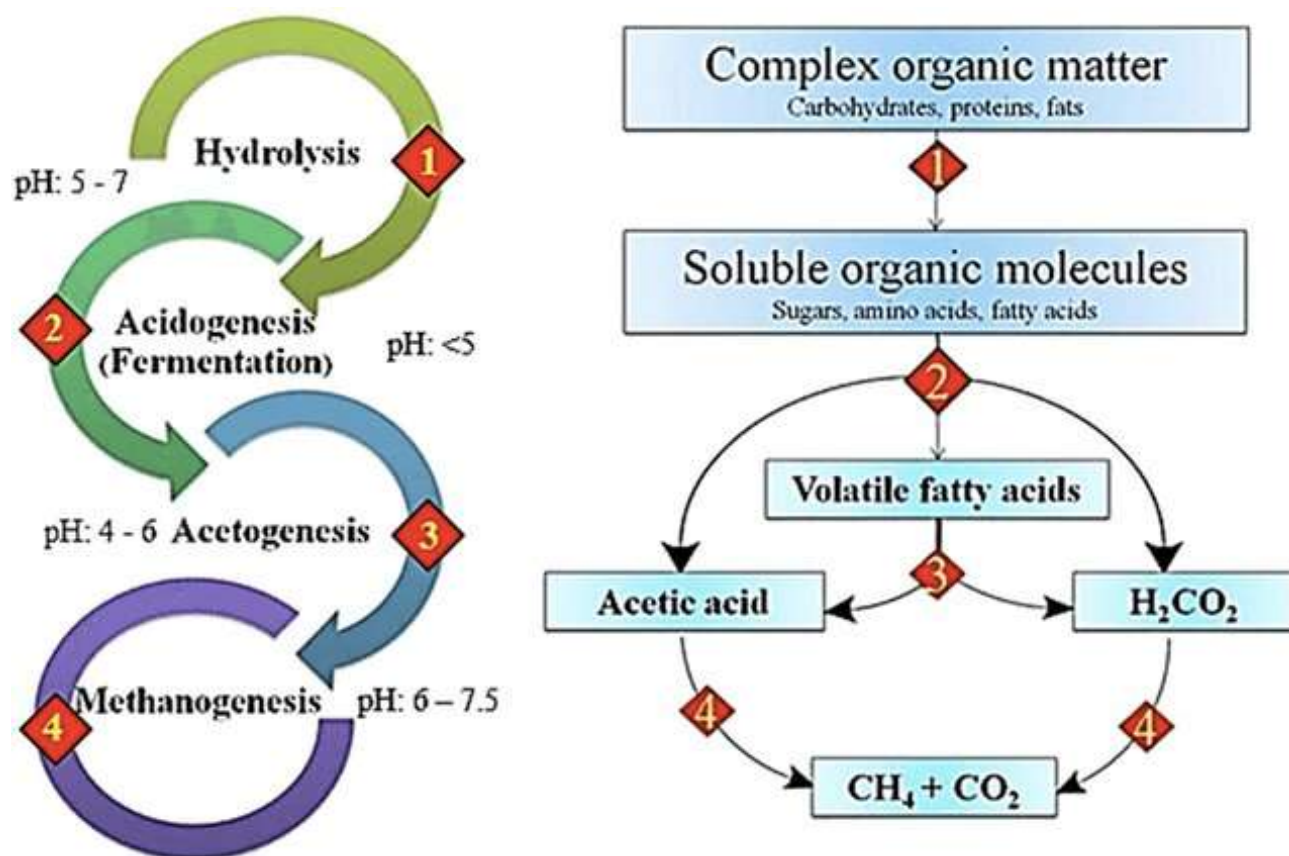


Figure 1. The Biochemical inter-conversion of OR during AD Treatment [3]

Whereas Fig 2 shows the application of AD to different types of OR. At another place, it is stated that AD is a natural process that occurs in oxygen free environment and is not accessible and interfered with human beings and hence used for the treatment of waste from the mid-1800s [4]. Furthermore, the AD process where biodegradable materials or organic refuse are break-downed in presence of different microbial population is basically based on the series of different stages such as hydrolysis, acidogenesis, acetogenesis, and methanogenesis [5]. Each stage is mathematically modeled by separate kinetic and mathematical models as shown in Table 1. Whereas various kinetic equations are applied to estimate

the performance of these microbes during AD biochemical decomposition of OR. However, these kinetic equations exhibit a pivotal role in understanding the behavior of bioreactors and the rate of biodegradation. In addition to this, these kinetic equations are applied to optimize the process parameters and in reactor designing. Thus, it is reported in literature that kinetic analysis is the best mathematical method to calibrate the biological treatment performance of any system and predict their performance [5].

sr	Model	Application	References
1	Pseudo-first Order	Substrate degradation	[6]
2	Monod kinetic model	Specific microorganism growth rate	[7]
3	Sigmoid Cone	Cumulative CH_4 calibration	[8]
4	Logistic Function	Calibration of cumulative CH_4 generation	[9]
5	Modified Gompertz model	Cumulative CH_4 calibration	[10]
6	ADM1 or Anaerobic digestion model 1	Employed to understand production biogas or methane process dynamics and its control and prediction.	[11]

Table 1. Various mathematical models are used in the process of AD of OR.

AD of organic refuse (OR) is carried out in multiple types of operating conditions with different types of bioreactors. These bioreactors include batch, continuous stir tank, complete mix, plug flow, and a hybridization of any of the above. Whereas the adoption and utilization of each bioreactor has its diverse advantages and disadvantages. The use of batch anaerobic bioreactor is more often, and this is because of its easy construction, operation and maintenance [12]. In literature, somewhere, it is stated that the biodegradation in AD process is mainly dependent on the different microbial species [5]. Moreover, about the importance of kinetic and mathematical studies, it is also revealed in literature that with the same process parameters and operational conditions, the results of kinetic studies which are achieved from experimental data could be replicated for estimating treatment efficiencies of full-scale biodigesters [13]. The one of the excellent examples available in the literature is the study conducted by Yilmaz (2003) on kinetic observations [14], where the authors have studied the suitability kinetic equations for five different ORs in the batch mode AD.

Therefore, it is witnessed from the literature that 19th century was the first century when the adaptation of kinetic study was done by Arrhenius and van't Hoff and the chemical kinetics was done by the authors [15]. Later in 1957 and 1972 were the years where the real application of kinetic models was applied for food processing [16, 17]. In continuation and in precedent year 1995, the kinetic modelling approach was applied to the physical and microbiological variations in any system [18]. However, a study performed in 2001 and that study has concluded and suggested some basic features of kinetic models. The study suggested that the kinetic models should be simple and have high goodness to predict experimental observations.

Furthermore, the AD process in literature also reported as to be carried out at two stages simultaneously such as hydrogenation and methanation [19]. For the calibration of these types of simultaneous processes, the International Water Association (IWA) has devised a robust mathematical model, and this is known as the Anaerobic Digester Model No 1 (ADM1) and reported in 2002 for the first time [19]. The suitable and appropriate selection of such these developed mathematical and kinetic models significantly

helping in identifying the best model for predication of biogas or methane generation along with organic fertilizers production for farmers and gardeners in same way [20].

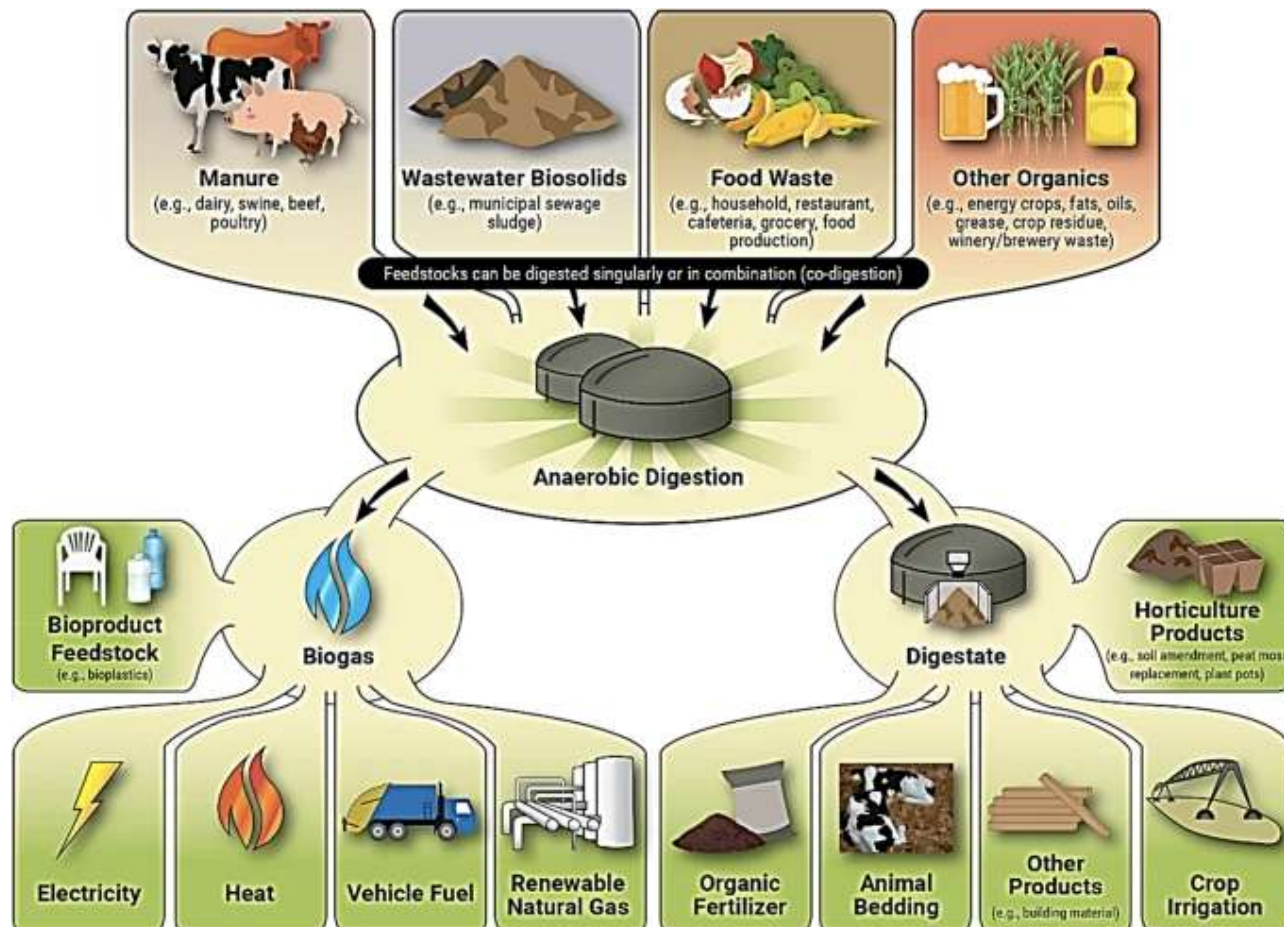


Figure 2. Utilization of organic refuse to produce bioenergy and other byproducts

Hence, this review paper presents the different mathematical and kinetic models used in AD processes. In addition to this, the paper gives more insights regarding the selection and suitability of mathematical models at the same time. Moreover, mathematical modeling helps in process control, trouble shooting, process optimization, design and scale-up. This review paper shall also discuss the application of each stated model in Table 1 discussed in the later sections below.

2 Modified Gompertz Model (MGM)

In literature, it is reported that the MGM kinetic model is suitable for predicting the biogas production in AD process as shown in the Eq. 1 [20].

$$Y_t = y_{me} \{ -e [R_{me} Y_m (\bar{\Delta} - 1) + 1] \} \quad (1)$$

In this study, the MGM was used to calibrate optimum yield of bioenergy (biogas) (y_m), optimum yield rate of biogas R_m , the lag phase of minimum time taken to generate bioenergy *gimel*. In this way, the study found the results respectively as optimum bioenergy generation ranges between 68 and 86 ml/g VS_{loaded} , 2.50–2.97 ml/g VS_{loaded} /day and 9.7–12.0 days (about 1 week 5 days) with finest goodness of fit ranging from 0.996 to 0.999 as described in the Eq. 2 and shown in the **Fig 3**. Hence, a mathematical equation was developed to describe the relationship between maximum biogas yield potential and volatile substrate concentration [20].

$$\Upsilon_m = -0.0266[VS]^2 + 4.8396[VS] + 129.1 \quad (2)$$

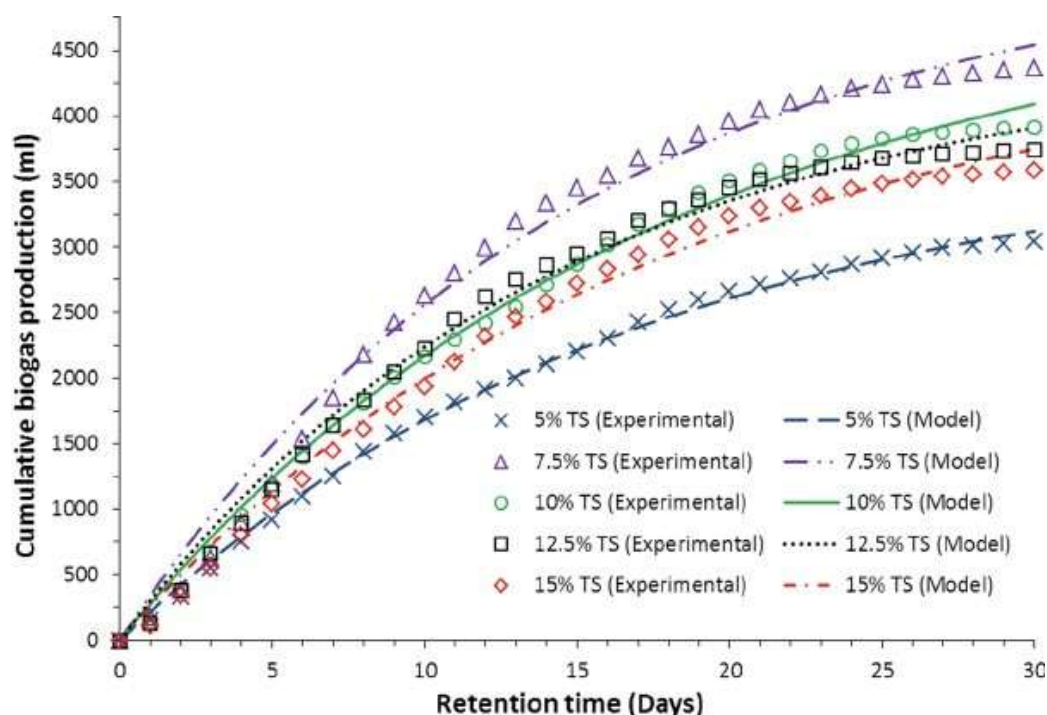


Figure 3. MGM model vs Experimental data plot

In another study the modified Gompertz model (MGM) was used to calibrate the experimental data using the parameters such as: y_m , R_m and λ . The estimation in this study was done by using the non-linear regression approach made possible by the Solver ToolPak of Microsoft Excel 2013. The MGM has fitted/predicted the experimental data with over 99% accuracy ($R^2 = 99.6 - 99.9\%$). Similar levels of accuracy were observed in the work of Syaichurrozi [21]. Furthermore, the MGM model was also applied under varying time and temperature conditions in food product process to demonstrate the surface inactivation behavior [22]. Where, the authors have studied the inactivation of microorganisms based on modification of conventional Gompertz model [23]. Thus, it is concluded that the varying temperature conditions were not properly demonstrated by the model and hence considered valid for isothermal conditions as given

below in Eq.3

$$\text{Log } N = \text{Log } N_0 - \text{Log} \left(\frac{N_0}{N_f} \right) e \left(-e \left(\frac{ke^1}{\log \left(\frac{N_0}{N_f} \right)} (L - t) + 1 \right) \right) \quad (3)$$

In this isothermal based model and MGM, the N stands for the density of microbial at a specific process time (t), L is for the time parameter (or shoulder), where k represents the maximum inactivation rate constant. N_0 and N_f are the initial and residual, respectively. Apart from all other mathematical parameters of cumulative biogas or its specific production, the duration of the lag phase (k) is also an important factor in determining the efficiency of AD treatment of OR. In this regard, mathematically 'k' can be calculated with the help of modified Gompertz mode as shown in Eq 4 [24].

$$C = B \exp \left\{ -\exp \left[\frac{R_b e}{B} (\bar{t} - t) + 1 \right] \right\} \quad (4)$$

Where, C = cumulative biogas production in mL;

T = time of digestion in days;

B = biogas potential of the substrate;

R_b = Optimum biogas production rate;

k = lag phase; and

$e = \exp(1)^{\frac{1}{4}} 2.7183$

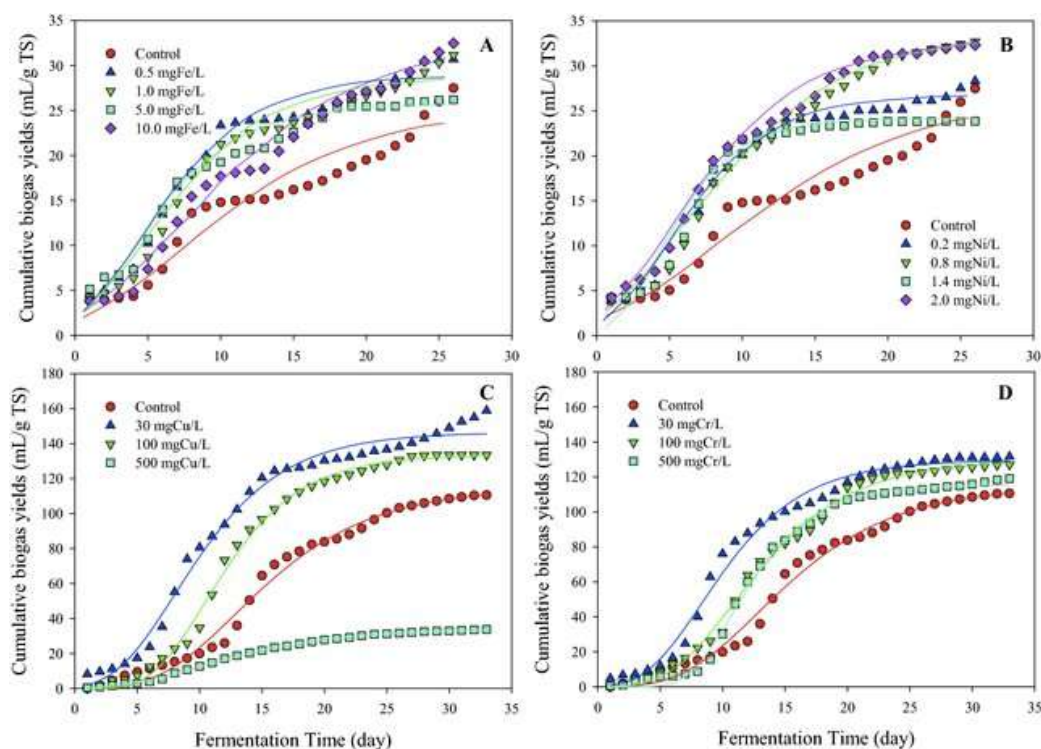


Figure 4. Two mathematical model predications vs. experimental observations [26]

In this research, it is summarized that MGM was found best model to describe cumulative biogas generation with more satisfying statistical curve fitting [24]. The same calibration of results prediction by MGM of biomethane generation was done as stated by Ali [25].

In another study conducted by Tian 2020 studied that the modified Sigmoidal models such as MGM and logistic growth models were used to investigate the kinetic evaluation of the bioenergy production potential while supplemented with heavy metals and describe the degradation patterns associated with varied heavy metal species and concentration [26] as shown in the Fig 4.

Furthermore, in the same study, both the mathematical models were able to represent the experimental results in the presence of heavy metals as shown by the no significant different correlation coefficients R^2 . Whereas the deviation between the MGM fitting results and experimental observations were quite less and best than the Logistic model. Hence, which suggests that the MGM is more suitable for describing the degradation patterns when AD of OR is carried out in the presence of heavy metals [26].

3 Logistic Model

Tian studied the kinetic evaluation of the biogas potential by using logistic growth model (LGM) to estimate the bioenergy and bio-decomposition patterns as given in Eq. 5 [26].

$$Y = \frac{A}{1 + B^{-R_{max}}} \quad (5)$$

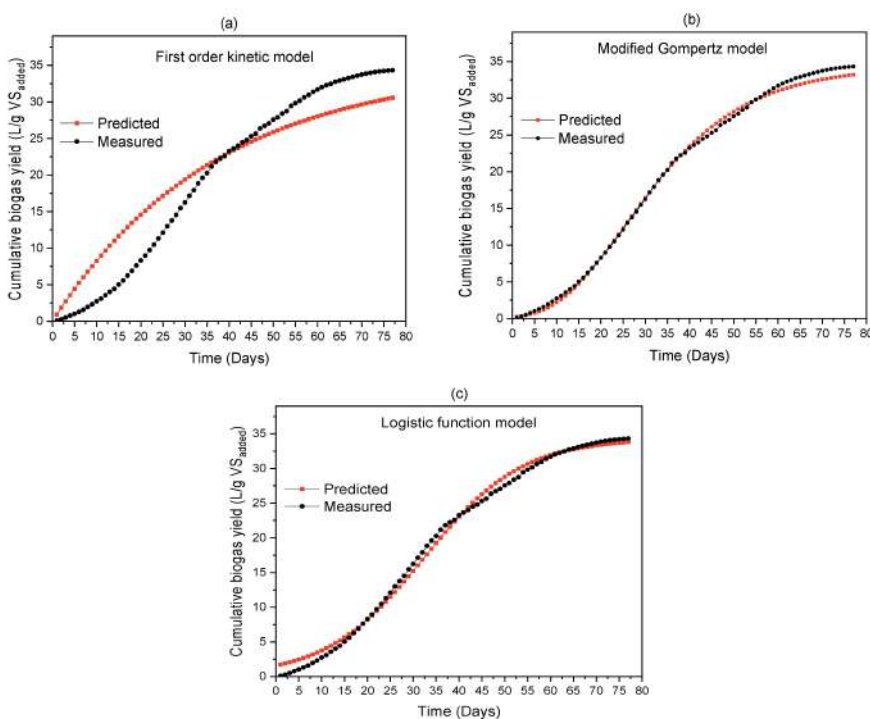


Figure 5. Modeled vs. experimental observation plot [27]

Food waste (FW) is the major fraction of the municipal solid waste (MSW) and it is generated in large quantity annually across the world and which poses serious environmental pollution and degradation [1].

To deal with global problems, a study was carried out on a large scale and used the 160 L anaerobic biofilm single-stage bioreactor for the treatment of FW [27]. In this study, three kinetic models were used such as MGM, LGM, and first-order kinetic model to describe and fit the cumulative biogas production potential from the experimental data. Hence, statistically it is concluded in this study that the MGM has best fit to calibrate experimental results among all three kinetic models as shown in Fig 5 [27].

4 Exponential Model

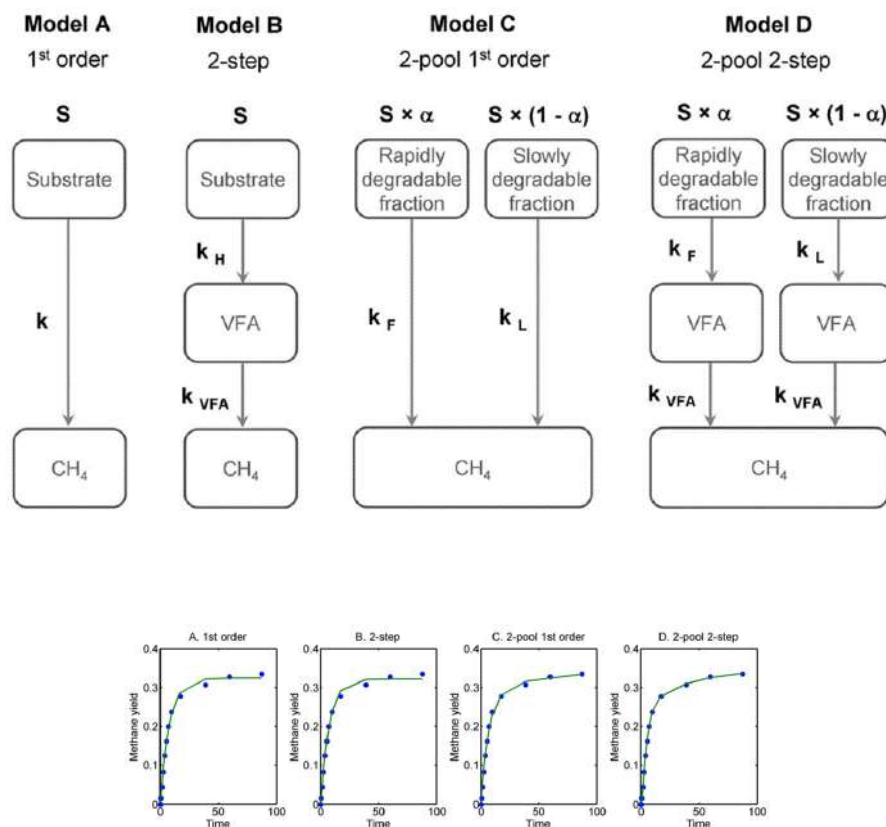


Figure 6. Optimization of experimental results through mathematical models [28]

Biochemical methane production curves are generally generated to provide handy information about the kinetics of substrate degradation, which is less time investigated [28]. Whereas, in the same study, it is reported that a basic comprehension of the kinetic models of the biogas process may be a first step towards a convergence of the assay methodologies on an international level. Hence in this regard a modeling toolbox containing an exponential model (EM) adjusted with a simple data-fitting method has been developed [28]. This kinetic EM should facilitate in (a) quality control of the biochemical reactions according to the goodness of fit of the model onto data series generated from the digestion of standard substrates, (b) estimate of the ultimate methane yield at infinite time (c) interpretation of substrate degradation kinetics

[28].

Hence, this research has revealed that Following this approach: four models were applied and implemented to evaluate kinetics of biomethane generation in batch mode AD; first order (Model A), two-step (Model B), dual-pool first-order (Model C), and dual-pool two-step (Model D) as shown in Fig 6 and Fig 7, respectively [28].

Model	Model type	Constants				
A	First-order	S	K			
		0.3239	0.1243			
B	First-order two-step	S	k_H	k_{VFA}		
		0.3212	0.1412	2.0410		
C	Dual-pool first-order	S	α	k_F	k_L	
		0.5108	0.5893	0.1372	0.0019	
D	Dual-pool two-step	S	α	k_F	k_L	k_{VFA}
		0.3460	0.7202	0.2365	0.0258	0.9044

Figure 7. Kinetic parameters obtained by various models

From Fig 6, it has been concluded that the dual-pool two-step model (Model D) has several positive outcomes such as it gives best data fitting and may estimate transitory accumulation of volatile fatty acids (VFA) in AD process. Thus, this revelation can be helpful, because the concentration of VFA in AD plays an important role in process success [28].

5 Anaerobic Digester Model No 1 (ADM1)

In AD of OR is considered as complex process, where mathematical and kinetic modeling can play an effective role in investigating the impact of various processes and operational variables on the efficiency of the treatment processes [29]. In this regard, the International Water Association (IWA) has developed a mathematical model, commonly known as the Anaerobic Digestion Model No. 1 (ADM1). Hence, this model was first practically applied to assess the performance of a full-scale AD of wastewater sludge. The experimental results and ADM1 simulated results are presented in Fig 8 [29].

From Fig 8, the model simulation results have good and close calibration of the most sensitive parameters with the experimental measured observations. Furthermore, in terms of effluent parameters such as chemical oxygen demand (COD) and effluent pH, the model performed reasonably well in predicting the process performance. However, some deviations were observed in biomethane production, which may be attributed to the non-homogeneity in the wastewater sludge composition or maybe depending on the degree of stabilization of the waste activated sludge (WAS)[29].

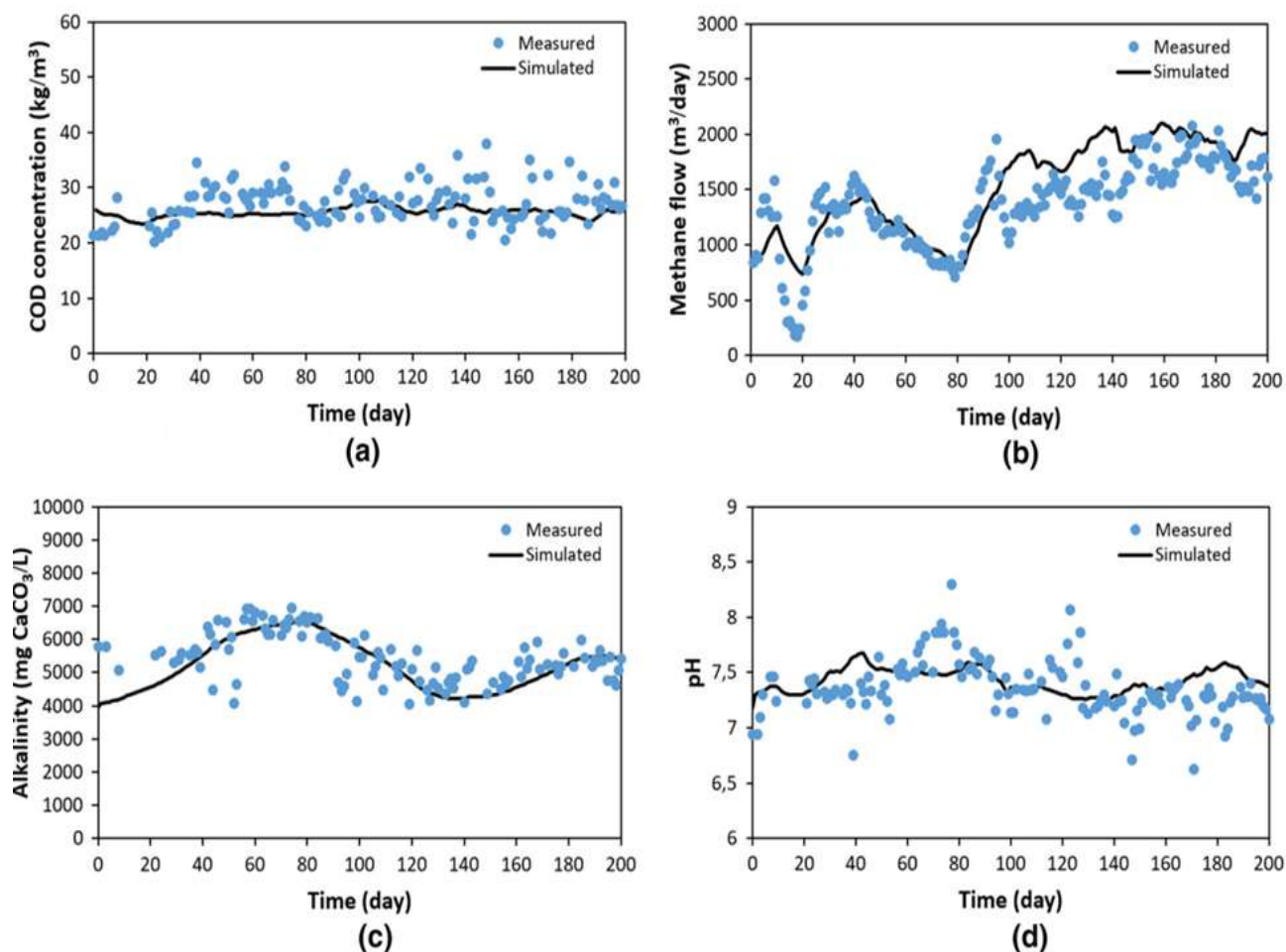


Figure 8. Model simulation results vs the different parameter of the AD process

6 Regression Model

In another research study, the regression model was used to determine the relationship and the impact of addition of nanoparticles (NPs) on the bioenergy generation [30]. For this purpose, single (variable or factor) multiple and linear regression models were utilized by using MS Excel 2016 (Microsoft, Redmond, WA, USA) [30]. Therefore, this model was generated to analyze the relationship between straight-line the four different variables. Hence, the generalized multiple regression estimates the β in the equation as given in Eq. 6:

$$Y = \beta_0 + \beta_1\chi_1 + \beta_2\chi_2 + \beta_3\chi_3 + \dots + \beta_n\chi_n \quad (6)$$

Herein, χ_n is the independent variable (IV), Y is the dependent variable, and β_s are the unknown regression coefficients. The goodness of the regression model was assessed by assuming a confidence interval $\alpha = 0.05$ of 95% as shown in Fig 9.

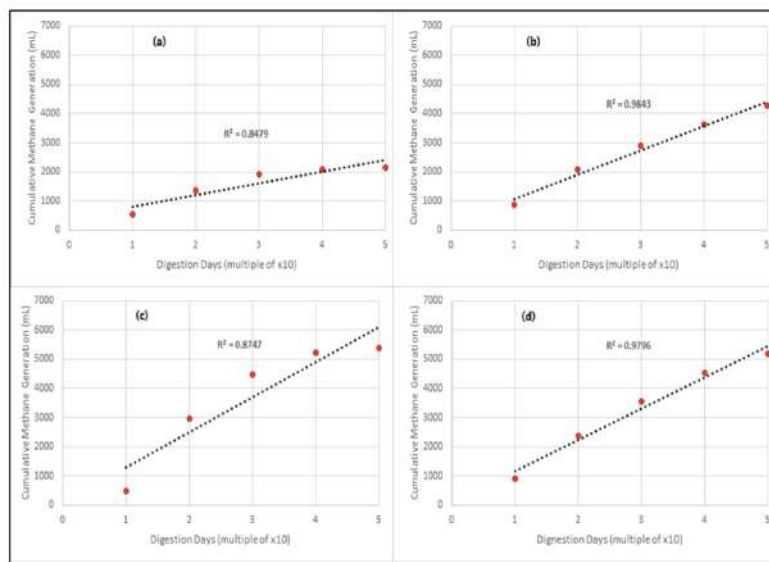


Figure 9. The simple linear regression plots

Moreover, the regression model as shown in Eq. 7 was also used to predict the biogas production as given in Fig 10 [31].

$$BGP = mx + c \tag{7}$$

Whereas BGP is biogas production in mL, m is slop of trend line, x is time in days, and c is the constant.

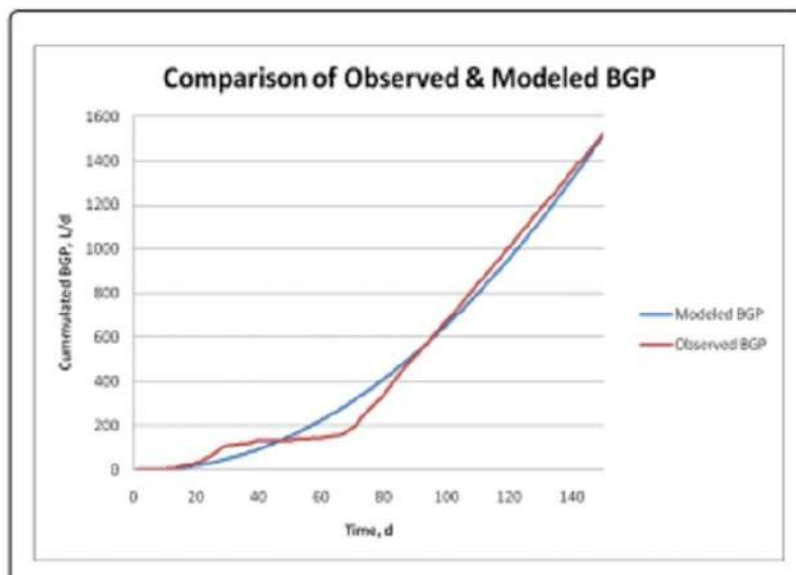


Figure 10. Model and experimental results calibration [31].

7 Conclusion

The mathematical modeling of anaerobic biodegradation of organic waste is always considered as the key catalyst of original research work. In this study, most successful mathematical models have been studied. Hence, it is found that all models have some limitations to adopt in every respect of the AD process calibration. But resultantly, this research reveals that the modified Gompertz model remains successful in defining the biogas or the methane production with more precision. Whereas the first order kinetic model has proved to be more successful in mathematically defining the biodecomposition rate of organic matters. This MGM is reported as the simplest and most accurate model for process designing and outcome estimations by the number of the researchers.

8 Author Contributions

Asim Ali :Conceptualization, methodology, write-up, **Hareef Ahmed Keerio**:Draft write-up, **Oshaque Ali Abro**: mathematical editing, **Muhammad Noor**:Draft review and paper formating, **Sallahuddin Panhwar**: Draft review **Rasool Bux Mahar**: Manuscript supervision and review in general.

9 Compliance with Ethical Standards

It is declare that all authors don't have any conflict of interest.

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