Review on anaerobic digestion models: Model classification & elaboration of process phenomena

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Abstract

Biogas is a well-established renewable energy source produced from anaerobic digestion (AD) of biomass/feedstock. It is probably the most versatile and efficient biofuel in terms of utilisable feedstocks and energy applications. To monitor, optimise, and control anaerobic digestion (AD), numerous mathematical models describing AD have been developed and reported. Although literature on the use of these models and their reviews have been published, their differences have not been collectively analysed and no generalised classification criteria for the models has been proposed based on such an analysis. This review covers most reported AD models, from the simplest linear equation capturing biogas production rate to complex Anaerobic Digestion Model No. 1. In addition to model classification and biochemical stages in AD, other processes like feedstock hydrolysis or mass and heat transfer essential to AD were discussed, analysed, and available models on them reviewed. This collective and comprehensive review approach has been undertaken to enable the evaluation of the interdependence of all processes, process factors, and process estimations and their individual, and interactive effects on AD.

Highlights

- Models of anaerobic digestion (AD) for efficient biogas production are reviewed.
- Review facilitates evaluation of interdependence of all processes involved in AD.
- Single-equation models are suitable for basic simulation and control.
- Complex models are advantageous when AD process is sensitive to intermediates.
- Further research in AD modelling should put more focus on the effect of stirring.

Keywords: Biogas, Anaerobic digestion, Single-equation model, Single-step degradation model, Multi-step dynamic model, AM2, ADM1, Mathematical modelling, Heat and mass transfer, Hydrolysis, Model classification, Microbial kinetics.

Word Count (<9900)

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List of abbreviations

Abbreviations	Meaning of abbreviations
AD	Anaerobic digestion
ADM1	Anaerobic Digestion Model No. 1
IWA	International Water Association
AM2	Acidogenesis-methanogenesis-two-steps
LCFA	Long-chain fatty acid
VFAs	Volatile fatty acids
TG	Thermogravimetry
BMP	Biomethane potential
SM	Schnute model
RM	Richard model
LM	Logistic model
TM	Transference model
SSDM	Single-step-degradation model
TSDM	Two-step-degradation model
MSDM	Multi-step-degradation model
HRT	Hydraulic retention times
CSTR	Continuous stirred tank reactor
FKM	First-order kinetic model
SBM	Surface-based model
GBM	Growth-based model

List of symbols

Symbols	Meaning of symbols
y	Biogas production rate or the total amount of biogas produced
k_{hyd}, α, a, b, c & k	Rate constant for dynamic and cumulative models
$\mathbb{a}$,$\mathbb{b}$, $\mathbb{c}$, and $\mathbb{d}$	Stoichiometric ratio
t_0, λ, τ, and t	Time of maximal biogas production rate, lag time, time constant, and instantaneous time
$\chi = V_t/V_\infty$	Fraction of biogas produced
V_t, and V_∞	Instantaneous, and total volume of biogas produced
m_i, m_t, and m_∞	Initial, instantaneous, and total volatile solid mass degraded
$\sigma, \beta, \varphi, \eta,$ and δ	Dimensionless shape factors or fitting factor
N , and n	Number of experimental runs and number of process factors or species being considered
A, and R_{max}	Biogas production potential, and maximal biogas production rate
ϕ , and ϑ	Material ratio, and kinetic constant
β_o, β_i, β_{ii}, and β_{ij}	Regression constants
x	Process factors, x (pH, concentration, temperature, etc.)
F,E, B, S, $\mathcal{I}$, $\mathcal{A}$, G, and G_D	Feedstock, enzymes, microbial biomass, substrate, intermediate, acetate, undissolved and dissolved biogas species concentration
$R_{\mathbb{J}}$	Reactive terms in the degradation process
μ, μ_{max} and K_d	Specific growth, maximum specific growth, and death rate of microbial species for computation of $R_{\mathbb{J}}$
R_E, $(K_L a)$, and K_H	Rate of evolution of biogas from liquid to gas phase, mass transfer coefficient, and Henry's constant for biogas species
Y, and K	Stoichiometric yield and reaction constant for computation of $R_{\mathbb{J}}$
$\mathcal{s}$ and $\mathcal{P}$	Collective degradable matter, and product formation for computation of Y
$\Sigma R_{\mathcal{s}}$	Summation of all reactions associated with $\mathcal{s}$

M,and $\mathbb{m}$	Molar mass and stoichiometric mole ratio
V_G, V_L, D, and $q_{o,G}$	Gas headspace volume, liquid volume, dilution rate, and biogas output flowrate of bioreactor
p_{atm}, p_j, and p_G	Atmospheric pressure and biogas species' partial pressure, vapour pressure inside the biogas bubble
R	Ideal gas constant
ρ, g, and γ	Liquid density, acceleration due to gravity, and surface tension of biogas bubbles in the liquid
k_p, and $(\psi_j^{o-vapour} - \psi_j^{o-liquid})$	Pipe resistance coefficient, and the difference of chemical potentials of biogas species, j
Z_i^+ and Z^+	Input and dynamic molar concentrations of cations
R_+, K_{a,CO_2}, and $(v_j\psi_j^o - v_j\psi_j^{o+} - v_j\psi_k^{o-})$	Cation production rate, dissociation constant for bicarbonate and summation of chemical ion potentials,
$D_{s,z}$ and $D_{s,r}$	Diffusivities in the axial, z and radial, r direction
h_L , and r_{BR}	Liquid level, and radius of the bioreactor
h_G, and r_G	Depth and radius of biogas bubble
I_j, K_I, and $\mathbb{I}$	Inhibition parameter of species, inhibition constant, and inhibition concentration
k_c, and k_s	Half-saturation coefficients for computation of μ
k_b, k_{CH}, k_1, and k_2	Kinetic parameters for computation of μ
S_0, and G_s	Initial substrate concentration and biogas production factor
pH_{ul} and pH_{ll}	Upper and lower pH limits
K_{mB}, and $\mathcal{E}$	Maintenance coefficient and activation energy
$\mathbb{A}$, and $\mathcal{B}$	Model constants for computation of temperature-dependent μ_{max}
T, T_{min} and T_{max}	Temperature, minimum and maximum temperature
K_{FH}, and K_{FS}	Rate constants of FKM and SBM for feedstock hydrolysis
K_M, and K_E	Half velocity constant and enzymatic rate constant for hydrolysis rate
Γ, m_F, and θ	Feedstock surface area, mass, and non-degradable fraction
Subscript, j & $j = 1, 2, \ldots, n$	Indicates the species or sequence being considered, typically S_j can mean LCFA or glycerol.
Subscript, i	Input, and typically the input composition of a substrate species, $S_j = S_{i,j}$

1. Introduction

Energy security and waste management are two recurring critical global security, economic and environmental issues that require persistent solutions. The interdependence of these two issues is highlighted when municipal and industrial wastes are converted into renewable energy. Biomass's contribution to the world's renewable energy is approximately 77% [1,2], and about 10% of the global energy supply [3]; of which biogas is the most versatile and efficient in terms of utilisable feedstocks and direct energy applicability.

Biogas is composed of approximately 50–75% methane (CH_4), carbon dioxide (CO_2), and impurities like 0–5% nitrogen (N_2), 0–5000 ppm hydrogen sulphide (H_2S), trace amounts of hydrogen gas (H_2), carbon monoxide (CO), and usually saturated with moisture (H_2O) [4]. It is produced through a complex multistep process - anaerobic digestion (AD) of organic matter. The amount and composition of biogas produced depend on the efficiency of the biochemical and mass transfer processes in each AD stage. These processes are influenced by factors like temperature, biogas species partial pressure, and pH. Therefore, mathematical models that relate these factors to feedstock, substrate, and intermediate utilisation, and the production of biogas, are required to monitor, analyse, optimise, and control AD stability [5–7].

Consequent to the preceding facts, numerous mathematical models have been developed to describe AD. These include the popular Anaerobic Digestion Model No. 1 (ADM1) [8], Gaussian, Gompertz, multi-regression, acidogenesis-methanogenesis-two-steps (AM2) models, etc. [9–12]. These models are uniquely different in their overall approach (mechanistic or statistical), initial assumptions, process phenomena, and the biochemical stages considered in their development. Although literature reviews on these models have been published, such differences have not been acknowledged. **Liang Yu et al.** [13], and **Ramachandran et al.** [14] reviewed ADM1 applicability, **Velázquez-Martí et al.**[15] elaborated on the exponential, Gompertz, transfer function models, etc. **Kythreotou et al.** [16] and **Gerber & Span** [17] detailed more on substrates and microbial kinetics. These review papers did not attempt to elaborate the general perspective on available AD/biogas models, analyse their specificity and similarity, and on such a basis deduce a classification approach for them. Although **Weinrich & Nelles** [18] (specifically for AMD1), **Manchala et al.** [19], **Simeonov & Stoyanov** [20], **Beuvink & Kogut** [21], and **Chezeau & Vial** [22] made positive contributions to resolving this issue, yet no comprehensive and clear comparative review exists. This issue when solved would facilitate appropriate comparisons of results from various biogas models - within and among the different classifications.

In addition to the biochemical stages in AD, other processes like feedstock hydrolysis, mass and heat transfers, and physicochemical processes are also essential to the model. This is because they enhance the robustness of AD models and make possible the evaluation of certain phenomena. Typically, in analysing the rate-limiting step in AD, modelling the hydrolysis, methanogenesis, and mass transfer of biogas is important, since one of them could be the slowest [23–27]. Furthermore, crucial - especially regarding the accuracy of AD models - are estimations of microbial activity parameters, microbe, and biogas yields, etc., and their dependence on process factors. Therefore, it is important to include these processes and estimations in a comparative review of AD modelling. Although there are review papers on this matter, most are focused on the stoichiometry of bioconversion, substrate, and microbial kinetics [16,17,24,28]. This collective and comprehensive review of all processes, process factors, and process estimations essential to AD, would enable the evaluation of their individual, and interactive effects on AD.

Therefore, this work seeks to review (theoretically and mathematically), classify, and evaluate AD models; independently and in comparison, to others based on their specificity, simplicity, accuracy, and applicability. In addition, to a collective and comprehensive review of all processes, process factors, and process estimations essential to AD. Most of the models and discussed processes are

illustrated with generic expressions allowing the development of an AD model appropriate for a specific application.

2. Description of anaerobic digestion

To reasonably discuss AD models, the stages in AD shall be briefly introduced, and for consistency and clarity, the reaction schemes in each stage shall be illustrated with lipid feedstock and its subsequent products. On a holistic level, AD is a simple process - although intrinsically, it involves four complex biochemical stages, and mechanical or chemical pretreatment may be required to enhance the utilisation of macronutrients [29]. These stages can be divided into: extracellular (pretreatment and hydrolysis stages) and intracellular stages (acidogenesis, acetogenesis, and methanogenesis)[29], and they occur both sequentially and concurrently via a group of microbes that metabolise feedstocks into biogas (mostly CH_4 & CO_2) in the absence of oxygen, see Fig. 1.

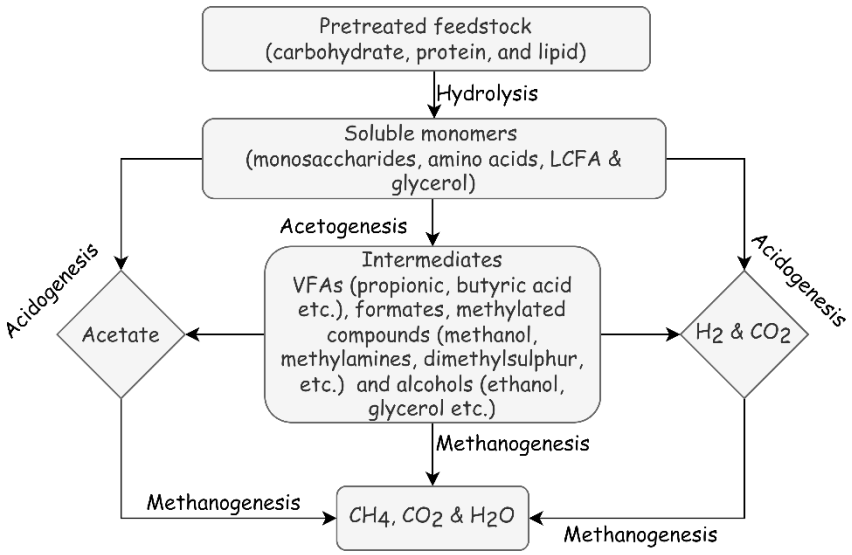


Fig. 1. Illustrative scheme of anaerobic digestion stages; LCFA – long chain fatty acids, VFA – volatile fatty acids

2.1. Feedstock hydrolysis

Feedstock hydrolysis has been reported as the rate-limiting step in AD [23–25], and is usually the reason why AD may experience long residence time, hence the need for its efficient implementation [29]. The hydrolysis rate depends on the type of macronutrients (e.g. biodegradation of amorphous cellulose occurs faster than crystalline cellulose [30]), substrate concentration, particle size, pH (optimum, 5-7), and temperature (optimum, 30-50 °C) [17,23].

$$C_{57}H_{104}O_6 + 3H_2O \rightarrow C_3H_8O_3 + 3C_{18}H_{34}O_2 \quad (2.1)$$

Hydrolytic/acidogenic bacteria are responsible for the hydrolysis of macronutrients (F) into substrates (S) via the production of extracellular enzymes - such as cellobiase (carbohydrates(F) into glucose(S)), proteases (protein(F) into amino acid(S)) and lipase (lipids(F) into glycerol and fatty acids (S)) [17,31,32]. Depending on the nature of the feedstock, the pretreatment and hydrolysis stages may be intertwined. Equation (2.1) illustrates the hydrolysis of lipid into glycerol and long-chain fatty acid (LCFA), respectively.

2.2. Acidogenesis of hydrolysis products

Acidogenesis is the fermentation of simple sugars (e.g. glucose), amino acids, and the anaerobic oxidation of alcohols (e.g. glycerol) and LCFA (e.g. oleic acid) by acid-forming bacteria [33,34]. Side

(e.g., CO_2, H_2O, H_2, and acetic acid) and intermediate products (e.g., propionic, butyric, valeric acid, etc., called volatile fatty acids, VFAs) are also formed. The acidogenic bacteria prefer degradation into acetic acid because these stages yield the highest energy and accelerate their growth (typically, a minimum doubling time of about 30 minutes), and can tolerate a pH value of 5-6 [17,35]. Although such rapid growth may inhibit the AD due to the decline in pH - especially when the acids are not metabolised quickly [36,37]. Note that acidogenesis can produce large amounts of CO_2 and H_2, especially with feedstock high in carbohydrates [38]. Equations (2.2) and (2.3) respectively illustrate the acidogenesis of LCFA (oleic acid) and glycerol without microbial activities (i.e. the synthesis of microbes ($C_5H_7O_2N$), energy for growth, and maintenance) [39].

$$C_{18}H_{34}O_2 + 16H_2O \rightarrow 9C_2H_4O_2 + 15H_2 \quad (2.2)$$

$$C_3H_8O_3 \rightarrow C_3H_6O_2 + H_2O \quad (2.3)$$

2.3. Acetogenesis of acidogenesis products

Acetogenesis is an intertwined subsidiary of acidogenesis. It involves the anaerobic oxidation of intermediaries (e.g. VFAs and alcohols) from acidogenesis to acetic acid and H_2 by acetogenic bacteria. Inhibition of the proceeding methanogenesis may occur if the H_2 produced is not quickly metabolised by methanogenic bacteria. The growth of acetogenic bacteria is slow, with a minimum doubling time of about 2 to 4 days [37,40,41].

$$C_3H_6O_2 + 2H_2O \rightarrow C_2H_4O_2 + 3H_2 + CO_2 \quad (2.4)$$

$$C_4H_8O_2 + 2H_2O \rightarrow 2C_2H_4O_2 + 2H_2 \quad (2.5)$$

Equations (2.4) and (2.5), respectively, illustrate the acetogenesis of propionic, and butyric acid into acetic acid, CO_2, and H_2, without microbial activities.

2.4. Methanogenesis of products from acetogenesis

Methanogenesis of organic matter to CH_4 from acetic acid (via the slow and low energy yield of acetoclastic methanogens, with a minimum doubling time of about 2-3 days), H_2, and CO_2 (via fast H_2-utilising hydrogenotrophic methanogens, with a minimum doubling time of about 6 hours) is well reported in literature [37] [41]. In addition to these groups, there are the formatotrophic, methylotrophic and alcoholotrophic methanogens which utilise formates, methylated compounds (e.g., methanol, methylamines and dimethylsulphur) and alcohols, respectively [37]. It should be noted that acetoclastic methanogens are sensitive to pH, nutrients, and trace element concentrations and account for about 70% of methane production [42]. In general, methanogens are AD "autopilot" because they control the alkalinity of the system via utilisation of acetic acid and CO_2. Hence, methanogenesis has been suggested as the rate-limiting step in AD, especially in conditions of high temperature, and soluble feedstock [23,26]. Equations (2.6) and (2.7) illustrate the methanogenesis via acetoclastic and hydrogenotrophic methanogens, equations for other groups can be found in [43].

$$C_2H_4O_2 \rightarrow CH_4 + CO_2 \quad (2.6)$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O \quad (2.7)$$

3. Model review on anaerobic digestion

The highlighted preceding stages of AD can be developed into a single-equation model and multi-step dynamic model, which are essential for simulation and control of the process as detailed in the ensuing subsections. These models are based on process factors (e.g. temperature, H_2 partial pressure, and pH) sensitive to AD. Therefore, it is important to understand how these factors affect the process, and such details have been elaborated [29,44,53,45–52].

3.1. Single-equation model

Single-equation models consider the holistic production of biogas from feedstocks without the various biochemical, mass transfer, and physicochemical processes. In these models, one equation describes biogas production, without interconnecting equations that describe the other highlighted processes.

3.1.1. Dynamic single-equation model

Dynamic single-equation models are designed to predict the biogas production rate ($mg \cdot g^{-1} \cdot time^{-1}$) from a given feedstock. The models are developed to describe changes in biogas production at each time step, via a simple-single analytical equation, rather than with a set of differential equations.

One of the reasons for dynamic models (single-equation or multi-step), is to apply them to process control [54,55]. The dynamic single-equation models are generic expressions that are not based on the AD principles, but on data trends, hence their constants do not have a biochemical meaning to the AD other than to curve fit the experimental data. Linear, exponential, and Gaussian models are typical examples of this type of model. More examples were reported and applied by **Barampouti et al.**[54]. In the linear model, Equation (3.1) [56], the biogas production rate, y ($mg \cdot g^{-1} \cdot time^{-1}$) increases linearly with the digestion time, t until it reaches its maximum production rate, after which there is a sudden linear decrease in production rate to zero. Therefore, its constants, a ($mg \cdot g^{-1} \cdot time^{-1}$) and b ($mg \cdot g^{-1} \cdot time^{-2}$) are of two values each, in order to model the linear increase and decrease regimes via two separate equations. Although this model is simple, the sharp initial increase and sudden decrease are not realistic. While in the exponential model, Equation (3.2) [56], the biogas production rate increases exponentially with time, t until it reaches its maximum, after which it decreases exponentially to zero. Its constants, a and b are of the same dimensions as in the linear model. The constant c($time^{-1}$) is positive or negative for the exponential increase or decrease regimes. In comparison to the linear model, the exponential model has been reported to be more realistic for the ascending regime; while the linear model is supposedly better for a descending regime [57,58]. **Ejimofor et al.**[58], **Veszelovszki et al.** [59] and **Pogaku et al.** [60] reported that biogas production rate simulated by the linear model showed better correlation than the exponential model.

$$y = a + bt \tag{3.1}$$

$$y = a + bexp(ct) \tag{3.2}$$

$$y = aexp(-0.5((t - t_0)/b)^2) \tag{3.3}$$

The Gaussian model, Equation (3.3) [56] is adequate for simulating biogas production rates in ascending and descending regimes with one equation. This model assumes that the biogas production rate follows a normal distribution [55]. The dimensions of its constants are similar to those of the linear and exponential models, where a ($mg \cdot g^{-1} \cdot time^{-1}$) and b ($time^{-1}$) are constants and t_0 is the time when the maximal biogas production rate occurs. **Das & Mondal** [55], **Lo et al.** [56] and **Ahmed & Kazda** [61] utilised and reported an adequate correlation of their AD data with the model.

3.1.2. Cumulative single-equation model

Cumulative single-equation models are developed to predict the total amount of biogas produced from a feedstock, y ($mg \cdot g^{-1}$) over a duration, t. Many cumulative models have been reported in literature: first-order kinetic, Gompertz, Schnute, transference function model, etc. Most of these models are non-linear and were developed based on the assumption of the rate-limiting step (e.g. microbial activity, hydrolysis rate, or biogas evolution rate) in the AD. Hence, these models (except the multi-regression model) can be appropriately termed, specific rate-limiting models. Cumulative models, unlike dynamic single-equation models, can be used to determine the following parameters: biogas production potential, maximum biogas production rate, and biogas production delay phase [62,63]. Therefore, they can be used to compare biomethane potential (BMP) as well as the biogas production rate in batch processes - modified Gompertz model is widely used for these purposes [64].

Zuru et al. [65] developed one of the simplest cumulative single-equation models - termed thermogravimetry (TG) kinetic model, based on the relationship between the fraction of biogas produced over a duration, t ,Equation (3.4). Where $= V_t/V_\infty$, V_t is the biogas volume generated over time, t and is proportional to the volatile solid mass degraded at that time, i.e. $V_t \propto (m_i - m_t)$ and V_∞, is the total biogas volume produced, and $V_\infty \propto (m_i - m_\infty)$, the volatile solid degraded over the entire process. Where m_i and m_∞ are the initial and total volatile solid mass.

$$\chi^{1/\sigma} = kt \tag{3.4}$$

It was assumed that biogas bubble nucleation and growth is the rate-determining step and that the value of σ describes the nucleation processes, with the value range, 2-4 being more applicable. Another simpler cumulative model is the first-order kinetic model, Equation (3.6). Where A is the biogas production potential (mg·g^{-1}) and k the first-order kinetic constant (time $^{-1}$). This model is based on the hypothesis that hydrolysis controls AD and that availability of substrate is the limiting factor [66].

$$y = A\{1 - \exp(-kt)\} \tag{3.6}$$

Bilgili et al. [67] and **Gioannis et al.**[68] reported a good correlation of this model with experimental data. It is assumed that the kinetic factor k is constant. However, during biogas production, process variables like microbial population change considerably with time and as such, this assumption is limited. Also, in cases where the biogas production shows delay, the model performs poorly, since it does not incorporate a delay factor [69].

The Gompertz model describes the cumulative biogas production curve in batch AD assuming the substrate concentration limit growth of microbes in a logarithmic relationship [70], Equation (3.7). The model was initially developed to describe microbe growth in batch mode [9,10]. However, for a better fit of experimental data, the modified Gompertz model, Equation (3.8) is often used [56][71]. Where R_{max} is the maximal biogas production rate (mg·g^{-1}·time^{-1}), $e = exp(1)$ and λ accounts for the latency phase (time). Although the true meaning of λ seems unclear [72]. **Lay et al.** [71] described the derivation of Equation (3.8).

$$y = Aexp(-exp(b - ct)) \tag{3.7}$$

$$y = Aexp\{-exp([R_{max}e(\lambda - t)/A] + 1)\} \tag{3.8}$$

Pramanik et al.[66] and **Achines et al.**[73] applied and compared cumulative models such as the first-order kinetic, modified Gompertz, logistic function, and cone models, and the results showed reasonable fit to the experimental data. However, **Pramanik et al.**[66] found that the modified Gompertz model was better as supported by **Zahan et al.**[74] and **Deepanraj et al.**[75].**Van et al.** [72] also utilised a cumulative biogas model, Equations (3.9) - (3.11) which can be considered a modified form of the Gompertz model. However, the constants in this model were deduced from a combination of equations solved simultaneously. Although the model is simple and robust, it is quite complicated - especially in the definition of factors. Where t_o is earlier defined and ϑ is a kinetic constant.

$$y = A\{1 - exp((\vartheta - 1)(t/t_o)^{1/\vartheta})\} \tag{3.9}$$

$$R_{max} = \{A/(e.\vartheta.t_o)\}exp(\vartheta).(1 - \vartheta) \tag{3.10}$$

$$A = \beta_o + \Sigma_{j=1}^{n}\beta_j\phi_j \tag{3.11}$$

Van et al. [72] used a linear regression model, Equation (3.11), that relates the biogas yield, A and material ratio, ϕ with Equation (3.9) and (3.10) to deduce A, R_{max} , ϑ and t_o.Where β_o and β_j in Equation (3.11) are the intercept and slope of the model and n, the number of different material ratio considered.

Other cumulative models reported in literature are given in Table 1. Where k_{hyd}, α, a, b, c & k are rate constants (time^{-1}), λ is the lag time, σ, β & δ are shape factors, and y_1 and y_2 are biogas produced at the time t_1 and t_2, respectively.

Table 1. Some popular cumulative biogas production models

Model	Expression	
Schnute model (SM) [76]	$y = y_1^{\beta} + \left(y_2^{\beta} - y_1^{\beta}\right)\{[1 - exp(-\alpha(t - t_1))]/[1 - exp(-\alpha(t_2 - t_1))]\}^{1/\beta}$	(3.12a)
Modified SM [77]	$y = R_m(1 - \beta)/\alpha\{(1 - \beta exp(\alpha\lambda + 1 - \beta - \alpha t))/(1 - \beta)\}^{1/\beta}$	(3.12b)
Richard model (RM) [78]	$y = a\{1 + \delta \exp[k(\tau - t)]\}^{-1/\delta}$	(3.13a)
Modified RM [79]	$y = A[1 + \delta exp(1 + \delta).exp\{(R_{max}(1 + \delta)/A)\,(1 + 1/\delta)\,(\lambda - t)\}]^{-1/\delta}$	(3.13b)
Logistic model (LM) [78]	$y = a/\{1 + exp(b - ct)\}$	(3.14a)
Modified LM [78,79]	$y = A/[1 + exp\{(4R_{max}(\lambda - t)/A) + 2\}]$	(3.14b)
Transference model (TM) [80]	$y = a\{1 - \exp(b - ct)\}$	(3.15a)
Modified TM [81]	$y = A\{1 - exp(-R_{max}(t - \lambda)/A)\}$	(3.15b)
Cone model [82]	$y = A/\left(1 + (k_{hyd}t)^{-\sigma}\right)$	(3.16)
Fitzhugh model [83]	$y = A(1 - exp(-kt)^{\sigma})$	(3.17)

The original or modified forms of the Schnute, Equation (3.12) [76,77,84], and Richard model, Equation (3.13) [76,78,85] were deduced based on microbial growth activity like the Gompertz, logistic, and transference function models - but with the inclusion of power factors to better account for different types of feedstocks, and to ensure a more accurate fit of experimental data, since this allows for flexibility in the shape of their curves [21,76,78]. From its derivation, the Schnute model is considered a generalised form of microbial growth activity models that includes, the first-order kinetic, logistic, Gompertz, Richards model, etc., and they can be deduced from it [64,76,84,86]. Furthermore, the Richard model based on the value of its fourth parameter ($\delta = -1, 0$ & 1), can be

reduced to the (transference, and first-order kinetic$\{\tau = 0\}$), Gompertz, and logistic models respectively [78].

The modified logistic model, Equation (3.14) gives a good prediction of the initial exponential increase and a final plateau at the maximal production level. It assumes the biogas production rate is proportional to the quantity of biogas already produced [66,87]. While the modified transference function, Equation (3.15) is a reactive curve-type model, based on control theory since it assumes that the biogas production process is a system receiving inputs and generating outputs, based on biogas yield from substrates [81,87]. The cone model, Equation (3.16) [82], assumes biogas production is dependent on the hydrolysis, and type of feedstock used, via the inclusion of a shape factor (σ) to account for the possibility of a lag phase. Consequently, this model is expected to correctly predict biogas yield from feedstocks with poor or heterogenous degradability [88–90]. Observation of Equations (3.16) and (3.17), the Fitzhugh model [83] shows some similarity, since, in comparison with other models, only two constants have biological/physical meaning, while the other parameter, σ, is a dimensionless shape factor used for better fitting of experimental data [91].

Cumulative models discussed thus far can be classified as exponential models (first-order kinetic, cone, Fitzhugh model, etc.); and sigmoidal models (Richard, Gompertz, logistic, transference model, etc. - in their original or modified form) [21,78,92,93]. Sigmoidal models are identifiable by the presence of a lag factor in their equations. While the exponential models have no lag factor and their data trends resemble curves with a negligible plateau at their ends, as illustrated by the curve of the first-order kinetic exponential curve in Fig. 2. Note that the reverse L-shape curve reaches its plateau faster than the exponential curve. Typically, the modified Gompertz model applies best to the degradation of simple organic substrates and adopts the reverse L-shape curve. While a complex substrate with heterogenous degradability resembles the elongated S-shape or stepped curve, and in this case models with flexible inflexion point like the Richards model with a fourth shape parameter are applicable [78].

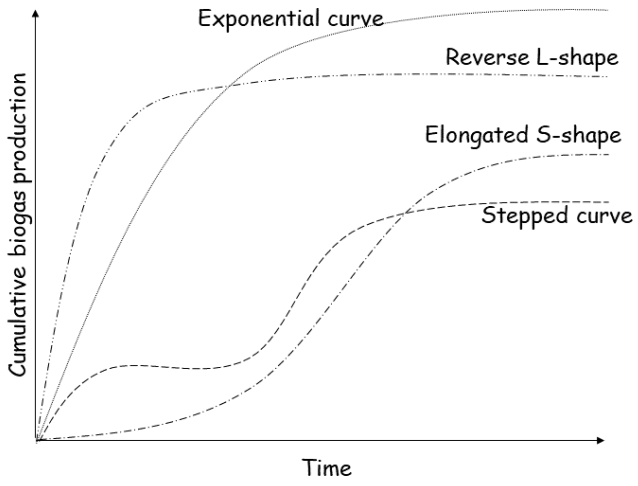


Fig. 2. Typical cumulative methane production curves[78]

Based on the preceding discussion, the criteria for choosing a cumulative model are dependent on the initial observation of plotted experimental data. While it may be clear to differentiate exponential and sigmoidal curves, the best model among exponential models would involve trial and error. Literature

reports on exponential models are shown in Table 2 [88,94,95]. Although regarding sigmoidal models, the modified Gompertz model is applicable to reverse L-shape curve [78,96]; however, for the elongated S-shape the logistic or transference model [96] can be chosen - based on trial and error, as suggested by **Li et al.** [81] and **Veluchamy & Kalamdhad** [97], Table 2. Finally, for the stepped curve, the Schnute or Richard models are suitable as supported by **Alizadeh et al**. [77] and **Ware & Power** [78], Table 2.

Although the works in Table 2 have used and compared exponential and sigmoidal models with each other, observation shows that the chosen cumulative model may have been influenced by the feedstock characteristic (i.e., degradability extent, feedstock heterogeneity, etc.), and operational conditions (e.g., feedstock pretreatment). This implies choosing a cumulative model requires prior analysis of experimental data.

Table 2. Literature on the degradation of feedstock to biogas

Observed literature	Feedstock & condition	Cumulative models used	Preferred model(s)
El-Mashad [88]	Switchgrass and Spirulina platensis algae	First-order kinetic, modified Gompertz, Fitzhugh, & cone models	Cone model best fitted the data
Cao et al. [94]	Untreated and pretreated sorghum bagasse	Fitzhugh, cone, monomolecular & modified Gompertz models	Cone & Fitzhugh models fitted better for untreated & pretreated feedstocks respectively
Zhao et al. [95]	Different fruit residues	First-order kinetic, modified Gompertz, cone & Fitzhugh models	Modified Gompertz and cone models fitted the data better
Alizadeh et al.[77]	Kitchen waste	Mitscherlich, Gompertz, modified Gompertz, logistic & Schnute models	Schnute and modified Gompertz models gave better fit
Cetinkaya & Yetilmezsoy [98]	Different agro-industrial substrates	Modified Gompertz, modified transference function, & modified logistic function models	Modified logistic function model fitted better
Ware & Power [78]	Complex poultry slaughterhouse wastes	Modified Richards, modified logistic, & modified Gompertz models	Modified Richards model fitted best
Li et al. [81]	Conventional thermal pretreatment of grass	Logistic function, modified Gompertz, & modified transference function models	Modified Transference function model gave the best fit

Zaidi et al.[99]	Microalgal biomass	Modified Gompertz & modified logistic models	Modified logistic function model fitted best
Zaidi et al.[100]	Green algae	Modified Gompertz & modified logistic models	Modified Gompertz fitted best
Veluchamy & Kalamdhad [97]	Lignocellulose pulp and paper mill sludge	Modified Gompertz & modified logistic, modified transference models	The modified Gompertz and logistic models had better fit

3.1.3. Multi-regression single-equation model

A multi-regression single-equation model is a multivariable equation that can be used to describe both dynamic and cumulative characteristics of biogas production, especially in cases when the exact mass transfer mechanism is unclear. This model in general can be a linear or nonlinear multivariable equation and can be simplified into a linear or nonlinear single-variable equation. **Das & Mondal** [55], and **Lo et al.** [56] utilised the linear single-variable equation, Equation (3.1). The generalised linear or nonlinear multi-regression single-equation model, Equation (3.18) may be deduced via design of experiment (DOE) with N number of experimental runs. Where $f(x)$ is the response i.e. biogas yield, x_j and x_j represent the process factors, x (pH, concentration of substrate, temperature, etc.), β_o is the model constant, β_j, the linear term, β_{jj}, the quadratic term, β_{jj}, the interactive term coefficient and n, the number of process factors [19]. **Motte et al.** [101] developed a multiple linear regression model to determine the impact of total solid (TS) content, inoculation ratio, and particle size of lignocellulosic biomass in AD.

$$f(x) = \beta_o + \Sigma_{j=1}^{n}\beta_j x_j + \Sigma_{j=1}^{n}\beta_{jj}x_j^2 + \Sigma_{j=1}^{n}\Sigma_{j=1}^{n}\beta_{jj}x_i x_j \quad (3.18)$$

Alternative to the Equation (3.18), is a form of nonlinear multi-regression single-equation model without interactive term and with the highest order ≥ the quadratic term, developed without DOE but based on curve-fitting of experimental data. This form of model is appropriately termed polynomial model, Equation (3.19), and it can also be used to predict biogas production in the form of dynamic and cumulative model. Where n and j =1, 2…, n are the order and order sequence of the polynomial model, β_o and β_j are the model constant, and coefficient of the independent variable, x, typically the amount of the specific feedstock. **Al-Wahaibi et al.** [102] utilised this model for the prediction of biogas and methane production from date fruit, rice waste, legume beans and food waste. **Abu-Reesh** [103] utilised the model for prediction of biogas from pretreated wheat straw.

$$f(x) = \beta_o + \Sigma_{j=1}^{n}\beta_j x^j \quad (3.19)$$

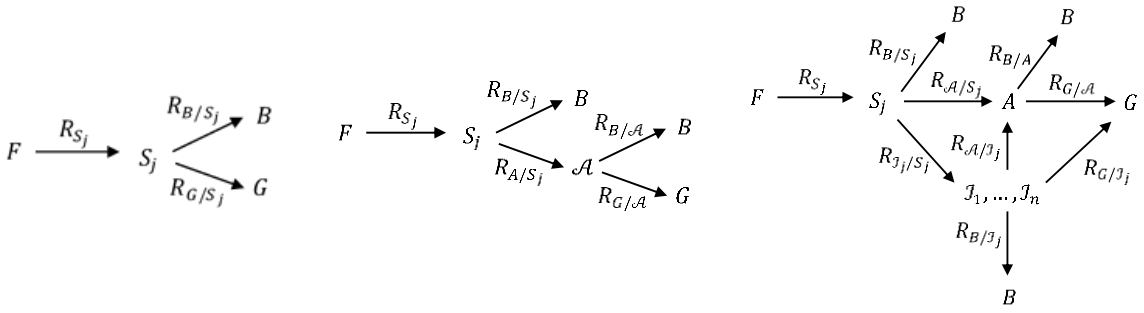
In summation of single-equation models, the dynamic single-equation models are not developed on AD principles, but on the mathematical relationship of experimental data trend. However, cumulative single-equation models are developed based on the assumed rate-limiting step; hence, their constants are meaningful to the AD, unlike dynamic single-equation models. Although dynamic single-equation models have meaningless constants – they are more appropriate for process control, since they predict the production rate rather than accumulative biogas yield. However, it should be noted that the effects of control factors like temperature, specific microbial activity, pH, etc. are not accountable in most single-equation models. This suggests that they may be inadequate for robust process control. Regarding the robustness of these models; while some models like thermogravimetry and first-order kinetic models assume constant kinetic factors, some others attempt an improved time-dependent kinetic factor for better experimental data prediction. The multi-regression single-equation model is

perhaps the most robust, since it is flexible and versatile during model development. This is because it can be designed as a dynamic or cumulative model and can incorporate the effect of all factors that affect AD. Therefore, in comparison to other models, better experimental data prediction is expected and consequently, this model would be more robust for process control [104]. Attempts have been made to improve the fit of single-equation models by incorporating them into multi-regression single-equation models. **Van et al.**[72] used the material ratio to develop a linear multi-regression single-equation model to estimate the biogas potential. **Mu et al.** [105] incorporated the solution of specific microbial growth rate deduced from the modified Gompertz model in the response of the DOE of AD factors (temperature, pH, and initial substrate to initial microbes ratio), to deduce the maximum specific microbial growth rate based on a nonlinear multi-regression single-equation model.

3.2. Multi-step dynamic model

The multi-step dynamic model accounts for a broad range of process phenomena involved in AD, using more than one sequentially interconnected dynamic equation. These equations among others include the dynamics of microbial growth, feedstock and the resulting substrate utilisation, biogas formation and evolution, etc., developed to predict the biogas production rate ($mg \cdot g^{-1} \cdot time^{-1}$) or ($mg \cdot L^{-1} \cdot time^{-1}$) from a given feedstock mass at any point in time, t. The simplicity or complexity of the model is dependent on how much detail is incorporated into it. In defining the nomenclature of this model, the term "multi-step" implies the stages and processes in the AD. While "dynamic" implies that these stages are described using a time-dependent differential equation.

Furthermore, the multi-step dynamic model can be grouped into three subcategories based on the substrate degradation level considered in the model, as illustrated in Fig. 3.: **single-step-degradation model (SSDM)**, considers the direct degradation of substrates (S_j, amino acids, sugars, LCFA & glycerol, etc. obtained from their respective feedstocks (F) composed of proteins, carbohydrates, lipids, etc.) into biogas (G); **two-step-degradation model (TSDM)**, considers the acidogenesis of substrates into acetic acid ($\mathcal{A}$) and methanogenesis of acetic acid into biogas; and **multi-step-degradation model (MSDM)** considers all substrate degradation levels, i.e. acidogenesis of a substrate to acetic acid and intermediates ($\mathcal{J}_j$, volatile fatty acids, alcohols, etc.), acetogenesis of intermediates, and methanogenesis of products from acidogenesis and acetogenesis into biogas. Note that some parts of the feedstock, substrates, and intermediates are converted into biomass (B). This type of dynamic model classification is similar to that suggested by **Simeonov & Stoyanov** [20], and analogous to the suggestion by Weinrich & Nelles [18] for AMD1. Note that $R_{\mathbb{J}} = R_{S_j}$,R_{B/S_j}, R_{G_j/S_j}, represent the reactive terms in the degradation process. Typically, for illustrative purposes, the reactive terms starting with B (e.g., R_{B/S_j}) represent the consumption rate of a given reaction component (e.g., substrate, S_j) into microbial biomass, B.



Single-step degradation Two-step-degradation Multi-step degradation

Fig. 3. Illustration of degradation steps considered in anaerobic digestion modelling; F – feedstock, S_j – j-th substrate, B – microbial biomass, G – biogas, A – acetic acid, J_j – j-th intermediate, $R_{\mathbb{J}} = R_{S_j}$, R_{B/S_j}, R_{G_j/S_j}, … – reactive terms in the degradation process

Different types of multi-step dynamic models also consider one or more of the following phenomena: hydrolysis of feedstock into substrates; physicochemical activities (such as dynamic equation to deduce pH); mass transfer from the liquid phase to the gas phase; and heat transfer in the AD process.

3.2.1. Single-step-degradation model

The SSDM is quite a simplified model. This model directly evaluates the biogas yield from the substrate, S_j. **Fedailaine et al.** [5] developed a SSDM that is both simple and suitable for control and found it capable of monitoring the progression and design of the AD system. Equation (3.20) illustrates the generic expression for this model. Note that the illustrative Equations (3.20) – (3.25) are based on a generalised continuous stirred tank reactor (CSTR) type bioreactor. Where $j = 1, 2, \ldots, n$ indicates the number of species being considered, i.e. various substrates, S_j (e.g. LCFA and glycerol from lipid feedstock, with input composition, $S_{i,j}$), intermediates, $\mathcal{I}_j$ (VFAs, alcohol, etc., with input composition, $\mathcal{I}_{i,j}$) and biogas constituents, G_j (e.g. CH_4, CO_2, H_2, etc.,) in the process. D is the bioreactor dilution rate (i.e. the inlet volumetric feed rate to liquid volume ratio).

$$dS_j/dt = D\left(S_{i,j} - S_j\right) + R_{S_j} - R_{B/S_j} - \Sigma_{j=1}^{n} R_{G_j/S_j} \tag{3.20}$$

3.2.2. Two-step-degradation model

The TSDM, also referred to as the AM2 model (acidogenesis methanogenesis, two-step model), is well suited for the control and design of software sensors [106] (due to its simplicity, i.e. lesser state variables, and parameters in comparison to MSDM), and AD monitoring [107]. In this model, the dynamics of the reaction of acetic acid, $\mathcal{A}$ is included with that of substrates, S_j, Equations (3.21) – (3.22). This model's performance is just as satisfactory in comparison to the reference AD model, ADM1 [106]. **Hill & Bart** [11], **Havlik et al.**[12], **Moletta et al.** [39], **Kiely G.et al.** [108], **Haugen et al.** [109], **Saeed et al.** [110], **Ma et al.** [111], etc. utilised and reported models that can be classified as TSDM. In general, these authors reported a satisfactory comparison of simulated and experimental data. **Hill & Bart** [11], specifically found that the TSDM was well within $\pm$10% of the experimental data and the stability of the process. **Kiely et al.** [108] performed sensitivity analysis of model parameters and suggested parameters that were the most and least sensitive to AD. **Flores-Estrella et al.**[112] and **Kil et al.**[113] used the TSDM model for AD control. Furthermore, **Alcaraz-González et al.** [114,115] showed that the TSDM model can support online control and optimisation [116].

$$dS_j/dt = D\left(S_{i,j} - S_j\right) + R_{S_j} - R_{B/S_j} - R_{\mathcal{A}/S_j} \tag{3.21}$$

$$d\mathcal{A}/dt = D(\mathcal{A}_i - \mathcal{A}) + R_{\mathcal{A}/S_j} - R_{B/A} - \Sigma_{j=1}^{n} R_{G_j/\mathcal{A}} \tag{3.22}$$

3.2.3. Multi-step-degradation model

A popular MSDM is the Anaerobic Digestion Model No.1 (**ADM1**), developed by **Batstone et al.** [8] in collaboration with the International Water Association (IWA). The **ADM1** is comprehensive [13], it incorporates dynamics for reactions of all intermediates, $\mathcal{I}_j$ (VFAs, alcohols etc.), in addition to that of acetic acid, $\mathcal{A}$ and substrates, S_j. Although **ADM1** is a robust model, it is complex, and numerical challenges may be expected in real-time implementation of state estimators and model-based controllers [109]. **Boubaker & Ridha** [117], and **Bornhoft et al.** [118], **Beschkov et al.** [119], **Keshtkar et al.** [120], **Balmant et al.** [121], etc. successfully utilised the MSDM. **Boubaker & Ridha** [117] used the modified ADM1 model for simulation and evaluation of parameters' sensitivity, and found good accuracy at different hydraulic retention times (HRT) and feed concentration. They concluded it can be used to improve the design and operation management of AD. This result was also supported by **Bornhoft et al.**[118], where it was suggested that ADM1 yielded qualitative results, especially when AD shows high sensitivity to one or more intermediates. **Haugen et al.**[109] noted ADM1 can result in poor biogas production predictions with temperature changes in the process; however, this can be improved by using the Arrhenius temperature function to express temperature dependent parameters or by adopting a similar approach [122,123]. While **Beschkov et al.** [119],

Keshtkar et al. [120], and **Balmant et al.** [121] used a specialised MSDM related to their processes. In addition, specific MSDM models incorporating temperature effects were successfully used for modelling of temperature phased AD [124,125], a process in which AD is realized in a series of reactors operated at different conditions. Equations (3.23) – (3.25) illustrate the generic expression of **MSDM**.

$$dS_j/dt = D\left(S_{i,j} - S_j\right) + R_{S_j} - R_{B/S_j} - R_{\mathcal{A}/S_j} - \Sigma_{j=1}^{n} R_{\mathcal{I}_j/S_j} \quad (3.23)$$

$$d\mathcal{I}_j/dt = D\left(\mathcal{I}_{i,j} - \mathcal{I}_j\right) + R_{\mathcal{I}_j/S_j} - R_{B/\mathcal{I}_j} - R_{\mathcal{A}/\mathcal{I}_j} - \Sigma_{j=1}^{n} R_{G_j/\mathcal{I}_j} \quad (3.24)$$

$$d\mathcal{A}/dt = D(\mathcal{A}_i - \mathcal{A}) + R_{\mathcal{A}/S_j} + R_{\mathcal{A}/\mathcal{I}_j} - R_{B/\mathcal{A}} - \Sigma_{j=1}^{n} R_{G_j/\mathcal{A}} \quad (3.25)$$

In summary of the multi-step dynamic model, while the MSDM & TSDM are comprehensive in accounting for the formation and utilisation of intermediates like acetate, propionic acid, etc. [17], their exact pathway for formation, breakdown, and measurement is ambiguous. Although the biochemical mechanism is clear on how intermediates and biogas are formed, depending on the operating conditions, microbe activity, feedstock characteristics, etc., the exact pathway followed in biogas formation is not certain and as such the contribution of each intermediate into biogas formation cannot be ascertained. As an illustration, consider the degradation of LCFA into acetate, accompanied with intermediates like propionic, butyric, valeric acids, etc., which are subsequently broken down into acetate, formate, etc., the process measurement of the acetate (used in modelling the dynamics of acetate) cannot quantify the amount of acetate formed directly from LCFA and those formed from the various intermediates. Likewise, the exact proportion of biogas formed from acetate and the reaction of hydrogen and carbon dioxide is not certain. Therefore, considering these uncertainties, it seems reasonable to directly deduce the biogas yield from the substrate via theoretical yield of the specific substrate (i.e., via the **SSDM**), collaborated with measured parameters from experimental analysis, to deduce the actual biogas yield. This approach allows for simpler, quicker, and adequate evaluation of unknown parameters, due to fewer number dynamic equations. In situations where the AD is not highly sensitive to one or more intermediates, MSDM & TSDM make for complexity rather than the accuracy of the simulated result. This is because the more dynamic equations for intermediates incorporated in the overall AD model, the more difficult its solution becomes and stiff in terms of resulting differential equations system [109,126]. However, for cases where AD is highly sensitive to one or more intermediates, the more detailed the description of intermediates' dynamics, the better the accuracy of the developed model. This preceding inference was highlighted by **Bornhoft et al.**[118] and, extensively, by **Arzate et al.**[127] for AM2 and ADM1. Based on this premise regardless of the complexity of MSDM & TSDM for these cases, they give better results than the SSDM. Therefore, it can be suggested that the magnitude of the difference in accuracy between MSDM, TSDM, and SSDM is dependent on the degree of sensitivity of AD to such intermediates.

Although TSDM & MSDM are expected to give accurate results, in developing and simulating such models, especially MSDM, many parameters need to be estimated and measured. However, such measurement may be unavailable, time-consuming, laborious, and expensive.

Furthermore, because some process variables negatively affect AD efficiency and stability, it is necessary to control the process. In general, dynamic models are popularly used for this purpose [5,106,109,128]. The dynamic single-equation, multi-regression single-equation, and multi-step dynamic models are such models. It has been reported that SSDM and TSDM are better as control models as opposed to MSDM. This conclusion was based on the degree of complexity and solvability of these models. **Fedailaine et al.** [5] for example, developed an SSDM due to its simplicity, and suitability for control. Also, the use of AM2 for control purposes (due to its tractable and fewer state variables), rather than ADM1 with numerous state variables and parameters was reported

[106,109,128]. **Sbarciog et al.**[129], and **Giovannini et al.**[130] used the AM2 for the control of hydrogen gas concentration, an important identifiable indicator of the stability of the AD process. Therefore, based on this premise, it is expected that the SSDM will be better for control purposes due to fewer equations and parameters as compared to the TSDM & MSDM models. In summation of the discussion thus far, in terms of the solvability, measurability, inaccuracy, and controllability of the AD the SSDM > TSDM > MSDM; while on the contrary, in terms of complexity, immeasurability, prediction accuracy, and uncontrollability MSDM > TSDM > SSDM.

4. Auxiliary process models and phenomena to multi-step dynamic model

In order to implement multi-step dynamic model, Equations (3.20) – (3.25), for a specific system, additional dynamics models, thermodynamic & physiochemical equations describing related phenomena have to be defined.

4.1. Reactive terms and microbial biomass dynamics

The reactive terms, $R_{\mathbb{I}}$, are dependent on the population, and kinetics of each microbial community in the AD. Therefore, it is important to model the dynamics of each microbial biomass, B_j as given by Equation (4.1).

$$dB_j/dt = D\left(B_{j,i} - B_j\right) + \mu_j B_j - K_{d,j} B_j \tag{4.1}$$

In literature, Equation (4.1) is developed separately for the degradation of the substrate and intermediate species and the formation of the different biogas species [8,117,118,120]. However, the various microbial species can be combined into a single model for each step in the AD (i.e. a model for microbes in the acidogenesis, acetogenesis, and methanogenesis steps separately) [121]. In other cases, a combined model for the acidogenesis-acetogenesis step and separately, for the methanogenesis step is used [11,12,129]. Finally, one combined model for all microbial species in the AD can be used [119]. Furthermore, it should be noted that a model for microbes in the hydrolysis step may not be required, because this is a result of enzymatic breakdown of the feedstock [17,31,32]. However, some authors considered this model for this step [108].

Having deduced B_j, the reactive terms, $R_{\mathbb{J}}$ can be estimated in relation to the specific microbial growth & death rate, (B_j, μ_j & $K_{d,j}$), and the stoichiometric yield, Y_j (i.e. the stoichiometric balance of biomass, B and product, $\mathcal{P}$ from the degraded substrate, $\mathcal{S}$, i.e. $Y_{B/\mathcal{S}}$ and $Y_{\mathcal{P}/\mathcal{S}}$) [5] or the reaction constant, K_j[111] – as given by Equation (4.2). Y_j, also known as the Monod yield, relates the use of degradable matter, $\mathcal{S}$ to microbial activities, i.e. $Y_{B/\mathcal{S}} = \Delta B/\Delta\mathcal{S}$, where $\mathcal{S} = S_j, \mathcal{I}_j$ & $\mathcal{A}$. It also relates degradable matter, $\mathcal{S}$ to product formation i.e., $Y_{\mathcal{P}/\mathcal{S}} = \Delta\mathcal{P}/\Delta\mathcal{S}$, where $\mathcal{P} = \mathcal{I}_j, \mathcal{A}$ & G_j. The stoichiometric yield, Y_j was used by **Kiely et al.**[108], **Andrew & Graef** [131] and **Fedailaine et al.**[5].While some other authors, e.g. **Beschkov et al.**[119], **Ma et al.**[111], **Sbarciog et al.**[129] etc. utilised the reaction constant, K_j. The exact definition of K_j is unclear, it could be a product of Y_j and μ_j , or a fitting factor, etc. Hence K_j may help limit the number of parameters to be estimated, however, it may have a meaningless biochemical definition, especially when considered as a curve fitting factor.

$$R_{\mathbb{J}} = f\left(B_j, \mu_j, K_{d,j}\ \&\ Y_j\right) \quad or \quad R_{\mathbb{J}} = f\left(B_j, \mu_j, K_{d,j}\ \&\ K_j\right) \tag{4.2}$$

4.2. Dynamics of temperature in anaerobic digestion

Although temperature is an important factor in AD, it is usually incorporated into temperature dependent parameters and not as a dynamic/state variable in most publications on AD models [123,132–135] etc. However, exception to this prevailing approach are reports by **Haugen et al.** [109],

Calise et al. [136] or **Alatiqi et al.** [137]. A temperature model is essential for the robust evaluation of temperature-dependent parameters such as mass transfer coefficients, pressure, specific microbial growth and death rates, and physicochemical properties of fluids. The temperature model can be deduced via the generic energy balance, Equation (4.3).

Input energy + Heat exchanger energy + Mixing energy + Reaction heat = Accumulation energy + Output energy + Water evaporation heat + Energy loss to the environment (4.3)

4.3. Biogas formation, evolution to headspace, and discharge from the bioreactor

Biogas is initially formed in the liquid phase before its evolution into the bioreactor gas headspace, Fig. 4. Hence, modelling these phenomena is important, since it enables the estimation of partial pressures of biogas components – especially of CO_2 and H_2. Specifically, CO_2 partial pressure is necessary for the pH estimation since dissolved CO_2 significantly influences the pH of the process [11,108,138] and high H_2 partial pressure negatively affects methanogenesis [139,140]. Therefore, controlling the pressure of CO_2 and H_2 (i.e., keeping them low) in the headspace would enhance AD efficiency and stability via their reduced solubility in the liquid phase.

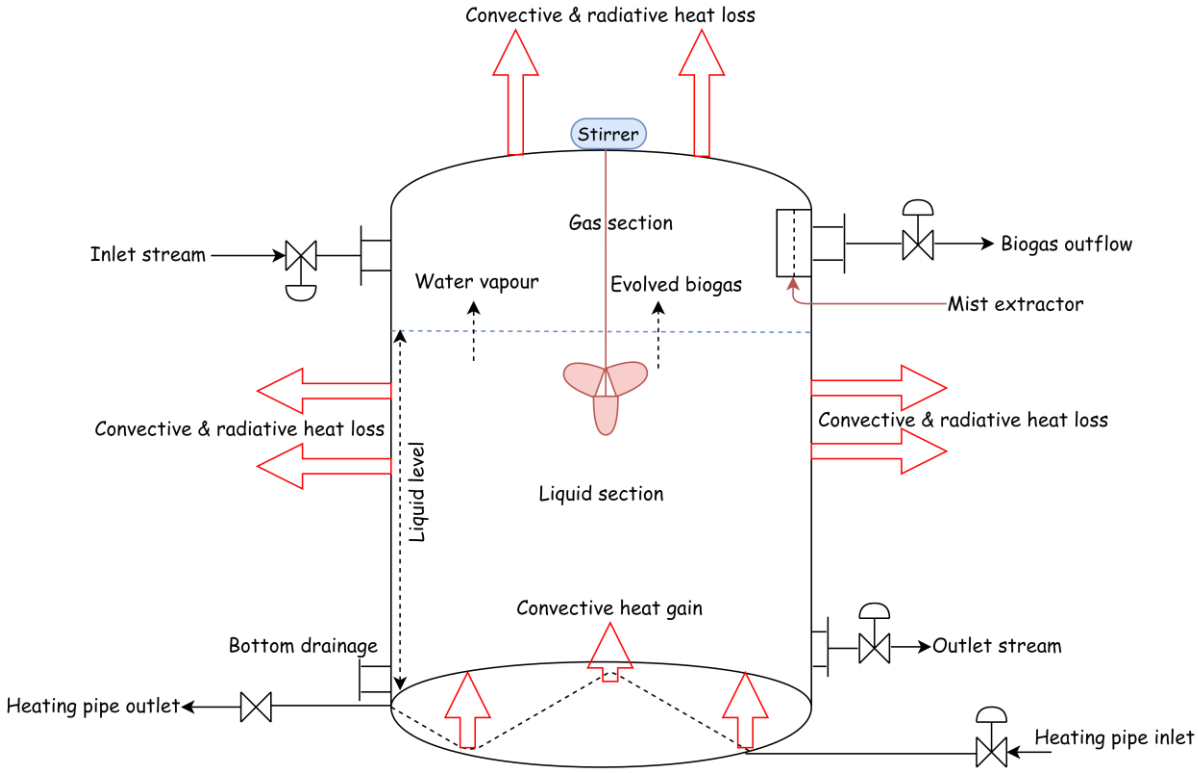


Fig. 4. Illustration of anaerobic digestion in a continuous stirred tank reactor (CSTR) type bioreactor with material and heat transfer

As regards the biogas formation rate, many authors (**Andrew and Graef** [131], **Batstone et al.**[8], **Giovannini et al.**[130], **Kiely et al.**[108], etc.) assumed that the gases formed are initially dissolved in the liquid phase as given by Equation (4.4), and then evolve based on Henry's law, Equation (4.5) via the gases partial pressure, Equation (4.7) as illustrated in Fig. 5. The resulting biogas species dynamics in the headspace are given by Equation (4.6). Where, $G_{D,j}$ is the dissolved biogas species, $R_{E,j}$, the rate of evolution of biogas from liquid to gas phase, $(K_L a)_j$, the mass transfer coefficient, $K_{H,j}$, Henry's constant for biogas species, R, the ideal gas constant, T, the temperature of the AD, V_G, the volume of gas headspace, V_L, the liquid volume, dn_j/dt, the molar dynamics of biogas species, dV_G/dt, the gas headspace dynamics and $q_{o,G}$, the biogas output flowrate. In contrast, **Ma et al.** [111],

Fedailaine et al.[5], **Beschkov et al.**[119] and **Sbarciog et al.**[129] considered the direct evolution of the biogas, given solely by Equation (4.4) but with the dilution and evolution rate expression, ($DG_{D,j}$ and $R_{E,j}$) $= 0$. Note that depending on the substrate degradation level, $\Sigma_{j=1}^{n} R_{G_j/I_j}$, $\Sigma_{j=1}^{n} R_{G_j/\mathcal{A}}$ and $\Sigma_{j=1}^{n} R_{G_j/S_j}$ may be zero. Typically for **SSDM,** $\Sigma_{j=1}^{n} R_{G_j/I_j}$ and $\Sigma_{j=1}^{n} R_{G_j/\mathcal{A}} = 0$, **TSDM,** $\Sigma_{j=1}^{n} R_{G_j/I_j}$ and $\Sigma_{j=1}^{n} R_{G_j/S_j} = 0$ and for **MSDM,** $\Sigma_{j=1}^{n} R_{G_j/S_j} = 0$.

$$dG_{D,j}/dt = -DG_{D,j} + \Sigma_{j=1}^{n} R_{G_j/I_j} + \Sigma_{j=1}^{n} R_{G_j/\mathcal{A}} + \Sigma_{j=1}^{n} R_{G_j/S_j} - R_{E,j} \quad (4.4)$$

$$R_{E,j} = (K_L a)_j (G_{D\,j} - K_{H,j} p_j) \quad (4.5)$$

$$dG_j/dt = (V_L/V_G) R_{E,j} - \left(G_j/V_G\right)\left\{q_{o,G} + (dV_G/dt)\right\} \quad (4.6)$$

$$dp_j/dt = (RT/V_G)\left\{dn_j/dt\right\} + \left(p_j/V_G\right)\{dV_G/dt\} \quad (4.7)$$

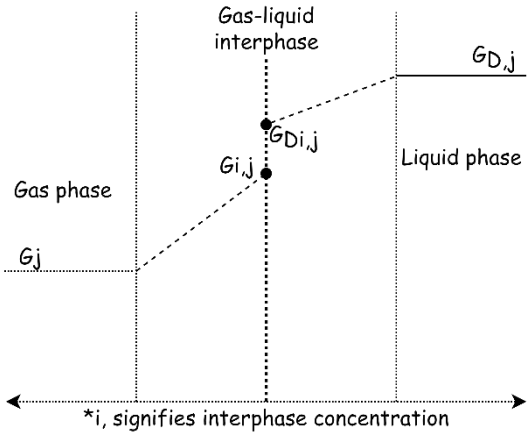


Fig. 5. Interphase mass transfer of biogas from a liquid substrate; G_j – j-th biogas specie, $G_{D,j}$ – j-th dissolved biogas specie

Mairet et al.[140] suggested that the biogas output flowrate, $q_{o,G}$ is dependent on the headspace overpressure as given by Equation (4.8). Where p_{atm} is the atmospheric pressure, $\Sigma_{j=1}^{n} p_j$, the total pressure of the process and k_p , the pipe resistance coefficient (pa·m^3·time^{-1}).

$$q_{o,G} = k_p(\Sigma_{j=1}^{n} p_j - p_{atm})\left(\Sigma_{j=1}^{n} p_j / p_{atm}\right) \quad (4.8)$$

$K_{H,j}$ estimation in AD was investigated by **Oh & Martin** [141]. According to the investigation, $K_{H,j}$ is the difference of chemical potentials, $-(\psi_j^{o-vapour} - \psi_j^{o-liquid})$ of each species, j in the liquid and gas phases, Equation (4.9).

$$K_{H,j}(g.L^{-1}atm^{-1}) = M_j exp\left\{-(\psi_j^{o-vapour} - \psi_j^{o-liquid})/RT\right\} \quad (4.9)$$

Based on the temperature reference of 298K, $(\psi_j^{o-vapour} - \psi_j^{o-liquid})$ of each species, $j = CH_4, CO_2$ & H_2 can be deduced respectively: 158.11, 75.44, and 173.7. Where R = 0.0821 L·atm·mol^{-1}·K^{-1}, M_j is the molar mass of biogas species and T (K), the temperature.

Biogas discharged from the bioreactor is usually high in water vapour (between 30 to 100g water per m³ gas). This results in reduced calorific value of the biogas unless the water content is reduced e.g. by drying [142]. Therefore, this implies the rate of consumption, formation, and evaporation of water in AD should be considered. **Taifouris** [143] developed a model to account for water in AD and **Draa** [106] considered the contribution of water vapour to the headspace or total pressure of the process.

The estimation of $(K_L a)_j$ in Equation (4.5) depends on the prevailing conditions in the bioreactor, for instance, the effect of stirring, liquid-gas interfacial area, and biogas bubbles size. A typical value of $K_{L,j}$ for sparged stirred fermentors and tower fermentors, is $3.5 \times 10^{-2} cm \cdot s^{-1}$ [144]. Adequate estimation of a_j may require detailed modelling of the bubble size distribution of biogas species. The idea of **Zuru et al.**[65] and **Hepworth** [145] can be used to estimate the biogas bubble radius (r_G) formed at depth (h_G), and with the vapour pressure inside the bubble (p_G) as given by Equation (4.10). While the **Mendelson's** correlation [146] for bubble velocity and the **Takahashi et al.** [147] correlation may be utilised for the estimation of a_j. Furthermore, the estimation of $K_{L,j}$ can be deduced via **Hikita et al.**[148] correlation of the Schmidt number for the desorption of gas from the free surface in a baffled agitated vessel under nonbubbling conditions, and the **Diaz et al.** correlation [149] for biogas diffusivity through a liquid.

$$p_G = p_{atm} + \rho g h_G + 2\gamma / r_G \tag{4.10}$$

Where P_{atm} is the atmospheric or surrounding pressure on the liquid phase, ρ, the liquid density, g, the acceleration due to gravity, and γ, the surface tension of biogas bubbles in the liquid.

4.4. pH estimation

The performance of AD is sensitive to changes in pH, which highlights the importance of modelling pH. Despite this fact, just as earlier noted for the temperature, some reports still consider pH as a parameter, rather than an independent or state variable [134,150,151]. **Hill & Bart** [11], and **Kiely et al.** [108] modelled pH comprehensively in similar procedure, Equations (4.11) - (4.14). A more detailed expression of Equation (4.11) is given by [152–154]. **Capris & Marais** [155] suggested an analogous approach for AD within a pH limit of 6.0 – 7.5. While the ADM1 by **Batstone et al.**[8] considered a more simplified approach based entirely on the formation and dissociation of carbonic acid, H_2CO_3 from CO_2 and H_2O.These pH models highlighted thus far are based on the dynamic model approach, and difference between them is the types of species considered in their charge balance (i.e. $HCO_3^-, HPO_4^{2-}, H_2PO_4^-, NH_4^+, VFA^+$, etc.). **Boutoute et al.** [156] utilized another approach – a numerical integration method, whose detailed analysis and comparison with dynamic model approach has been elaborated by **Campos & Flotats** [153]. In Equations (4.11) - (4.14), Z_i^+ and Z^+ are the input and dynamic molar concentrations of cations not affected by biochemical reaction (e.g., Na^+, Ca^+ etc.), $[NH_4^+]$, the molar concentration of ammonium as a result of this microbial activity and the breakdown of protein in feedstock and S_j, the concentration of free fatty acids (FFAs), VFAs and other acids (e.g., amino acid). While M_{NH_4}, and M_{S_j} are the molecular weights of ammonium and acids. R_+, the cation production rate other than ammonia and hydrogen (obtainable via the expression similar to Equation (4.1) [11]) and K_{a,CO_2}, the dissociation constant for bicarbonate, HCO_3^- based on ionic equilibrium with CO_2[11,108].

$$[HCO_3^-] \cong Z^+ + [NH_4^+]/M_{NH_4} - \Sigma_j (S_j / M_{S_j}) \tag{4.11}$$

$$dZ^+/dt = D(Z_i^+ - Z^+) + R_+ \tag{4.12}$$

$$[H^+] = K_{a,CO_2}([CO_2]/M_{CO_2})/[HCO_3^-] \tag{4.13}$$

$$pH = -\log_{10}[H^+] \tag{4.14}$$

The K_{a,CO_2}can be deduced as proposed by **Oh & Martin** [141] based on ionic equilibrium with species, $j = CO_2$ in AD, Equation (3.37). Where $\not{j}$ and $\not{k}$ are constituent ions of specie, j.

$$K_{a,j} = exp\left\{(\upsilon_j \psi_j^o - \upsilon_{\not{j}} \psi_{\not{j}}^{o+} - \upsilon_{\not{k}} \psi_{\not{k}}^{o-})/RT\right\} \tag{4.15}$$

Based on temperature reference of 298 K the summation of chemical ion potentials, $(\upsilon_j\psi_j^o - \upsilon_{\acute{\jmath}}\psi_{\acute{\jmath}}^{o+} - \upsilon_{\acute{k}}\psi_{\acute{k}}^{o-})$ can be deduced as, -358.83. Where R = 0.0821 L·atm·mol^{-1}·K^{-1} and T (K), the temperature.

4.5. Influences of stirring in anaerobic digestion

The preceding facts and models assume that the concentration and temperature of AD are homogeneous within the bioreactor's coordinates, however, this is not true in practice, especially for large bioreactors, hence the need to discuss the effect and modelling of stirring operation. Stirring enhances the AD, via homogeneity in the mass transfer processes (e.g., adequate contact between microbes and substrate), pH and temperature, etc. **Hemrajani & Tatterson** [157] describes the dynamics of homogeneity in stirring operation. Stirring also enhances the dissolution of gas bubbles, prevents foaming, clogging in the bioreactor, etc. [51,53]. However, it should be noted that microbes are sensitive to mixing intensity and are stressed by excessive mixing [50]. **Vavilin & Angelidaki** [158] incorporated axial and radial fluid distribution (via the Navier-Stokes equation) on substrates, Equations (3.20, 3.21 & 3.23) and biomass, Equation (4.1) models as illustrated in Equation (4.16) to account for the effect of mixing. This analogy is also applicable to acetate and intermediates models, so c is defined as the concentration of substrate, S_j, acetate, $\mathcal{A}$, interme diate, $\mathcal{I}_j$ and biomass, B. Where $D_{\mathcal{s},z}$ and $D_{\mathcal{s},r}$ are diffusivities in the axial, z and radial, r direction of the liquid level, h_L and the radius of the bioreactor, r_{BR}, and $\Sigma R_{\mathcal{s}}$ is the summation of all reactions associated with the given $\mathcal{s}$. The Navier-Stokes equation is also applicable to the temperature dynamics.

$$d\mathcal{s}/dt = D_{\mathcal{s},z}(d^2\mathcal{s}/dz^2) + D_{\mathcal{s},r}[\{1/r\}d/dr(rd\mathcal{s}/dr)] + D(\mathcal{s}_i - \mathcal{s}) + \Sigma R_{\mathcal{s}} \quad (4.16)$$

5. Biochemical kinetics phenomena and parameters

Regarding Equation (3.26), the calculation of $R_{\mathbb{J}}$ requires the estimation of parameters like μ_j , $K_{d,j}$ and Y_j, which may be dependent on process factors such as concentration, pH, and temperature, as discussed in this section.

5.1. Microbial activity and inhibition

Different empirical models have been developed for microbial specific growth rate, μ based on its dependence on temperature, pH, concentration, etc. The Monod equation is the simplest model for μ, other alternatives are listed in Table 3. However, microbes do not attain their full potential (i.e. maximum specific growth rate, μ_{max}) due to inhibition, I_j caused by substrate, product, pH, and temperature, etc., hence inhibition factors are usually incorporated into the μ model as illustrated in Equation (5.1), based on the Monod equation [8,22].

Monod model with inhibition	$\mu = \mu_{max}\frac{S}{K_S + S}\Pi_{j=1}^{n} I_j$	(5.1)
Non-competitive inhibition	$I_j = \frac{1}{(1 + \mathbb{I}/K_{I,j})}$	(5.2)
Competitive inhibition	$I_j = \frac{1}{(1 + \mathbb{I}/S)}$	(5.3)
Limitation model	$I_j = \frac{1}{(1 + K_{I,j}/\mathbb{I})}$	(5.4)

Where $\mathbb{I}$, is the inhibitor concentration, and $K_{I,j}$, the inhibition constant (a measure of inhibitor concentration that reduces the microbial growth to 50% it's μ_{max}) of species j= substrate, product, and pH. The definition of I_j for non-competitive and competitive inhibition parameters are given by Equations (5.2) and (5.3). Although there is another form of inhibition termed limitation - caused by

secondary substrate, Equation (5.4). An identifiable limitation in AD is that of substrate consumption caused by build-up of ammonia formed along with microbes synthesis [8]. Competitive inhibition applies to multi-substrate systems (i.e., main, and secondary substrates) e.g. (LCFA & glucose), (butyrate & valerate), etc. This can be modelled by combining Equations (5.1) and (5.3), or by Equation (5.5) [159]. In Equation (5.5), Equations (5.2), and (5.4) can be applied, to incorporate non-competitive inhibition and limitation respectively, but not Equation (5.3). Also available is the special uncompetitive model, Equation (5.6) [160], for which Equations (5.2), (5.3), and (5.4) can be incorporated.

Monod model with competitive inhibition

$$\mu_S = \mu_{max} \frac{S}{K_S(1 + \mathbb{I}/K_{I,j}) + S} \Pi_{j=1}^{n} I_j \quad (5.5)$$

Monod model with uncompetitive inhibition

$$\mu_S = \mu_{max} \frac{S}{K_S + S(1 + \mathbb{I}/K_{I,j})} \Pi_{j=1}^{n} I_j \quad (5.6)$$

A typical definition of inhibition factor based on the main substrate, S (i.e., non-competitive inhibition, j & $\mathbb{I} = S$), is $I_S = 1/(1 + S/K_{I,S})$. $K_{I,S}(g/L)$ is the inhibition parameter. Applying the expression, I_S to Equation (5.1), yields the **Haldane (1930)** model. However, not every model applies the substrate inhibition via the combination of Equation (5.1), and Equations (5.2) - (5.4). A simple modification is the **Grant (1967)** model. The **Andrews (1968)** model utilized the uncompetitive model, Equation (5.6) for self-induced inhibition of a substrate, i.e., j & $\mathbb{I} = S$, so that $(1 + \mathbb{I}/K_{I,j}) = (1 + S/K_{I,S})$. The **Haldane (1930)** approach was adopted by the **Ierusalimsky (1967)** model for product inhibition. Alternative product inhibition approaches are the **Holzberg et al. (1967)** and **Aiba et al. (1968)** models.

Table 3. Summary model for specific microbial activity [17,19]

Model	Specific microbial activity	Details
Monod (1949) [161,162]	$\mu = \mu_{max} \frac{S}{k_s + S}$	k_s is the half-saturation coefficient
Moser (1958) [163,164]	$\mu = \mu_{max} \frac{S^{\varphi}}{k_s + S^{\varphi}}$	
Contois (1959) [164,165]	$\mu = \mu_{max} \frac{S/B}{k_c + S/B}$	k_c is the half-saturation coefficient for s/B
Chen and Hashimoto (1979) [166]	$\mu = \mu_{max} \frac{S/S_0}{S/S_0 + k_{CH}(1 - S/S_0)}$	S, and S_0 are the substrate and initial substrate concentration k_{CH} is a kinetic parameter
Bergter (1983) [167]	$\mu = \mu_{max} \frac{S}{k_s + S}\{1 - \exp(-t/\lambda)\}$	λ is the lag time of the process
Mitsdoerffer (1991) [168]	$\mu = \mu_{max} \frac{S^{\varphi}}{S^{\varphi}(1 + G_s k_b S^{\varphi})}$	G_s is the gas production factor ($L \cdot g^{-1}$) k_b is a kinetic parameter
Substrate inhibition model		
Haldane (1930) [169,170]	$\mu = \mu_{max} \left(\frac{S}{k_s + S}\right)\left(\frac{k_{I_j}}{k_{I_j} + S}\right)$	k_{I_j} is substrate, $j = S$ inhibition parameter due ($g \cdot L^{-1}$)
Andrews (1968) [171–173]	$\mu = \mu_{max} \frac{S}{k_s + S + S^2/k_{I_j}}$	

Grant (1967) [174]	$\mu = \mu_{max} \frac{1}{k_{I_j} + S}$	
Product inhibition model		
Ierusalimsky (1967) [175]	$\mu = \mu_{max} \left(\frac{S}{k_s + s}\right)\left(\frac{k_{I_j}}{k_{I_j} + S}\right)$	k_{I_j} is the product, $j = P$ inhibition parameter (g·L^{-1})
Holzberg et al. (1967) [176,177]	$\mu = \mu_{max} - k_1(P - k_2)$	k_1 & k_2 are kinetic parameter (g·L^{-1})
Aiba et al. (1968) [178,179]	$\mu = \mu_{max} \left(\frac{S}{k_s + S}\right) exp(-k_{I_j}.P)$	P is the product concentration

Microbes at each stage in AD perform best within certain pH ranges. Therefore, it is important to consider pH inhibition on microbial activity via a pH inhibition factor applicable to Equations (5.1), (5.5), and (5.6). Typical pH inhibition factors utilised in literature are given in Equations (5.7) – (5.10).

$$I_{pH} = \frac{1 + 2(10^{0.5(pH_{ll} - pH_{ul})})}{1 + 10^{(pH - pH_{ul})} + 10^{(pH_{ll} - pH)}} \tag{5.7}$$

$$I_{pH} = \exp\left\{-\eta\left(\frac{pH - pH_{ul}}{pH_{ul} - pH_{ll}}\right)^2\right\} \begin{matrix} pH < pH_{ul} \\ I_{pH} = 1, pH \geq pH_{ul} \end{matrix} \tag{5.8}$$

$$I_{pH} = \frac{[H^+]}{K_{[H^+]} + [H^+] + [H^+]^2/K_{I,[H^+]}} \tag{5.9}$$

$$I_{pH} = \frac{K_{pH}^{\varphi}}{K_{pH}^{\varphi} + [H^+]^{\varphi}}; \varphi = \frac{\eta}{pH_{ul} - pH_{ll}}; K_{pH} = 10^{0.5(pH_{ul} - pH_{ll})} \tag{5.10}$$

Where pH_{ul} and pH_{ll} are the upper and lower pH limits at which microbes are inhibited, and η is a constant. **Zwietering et al.**[180] and **Batstone et al.**[8] suggested, $\eta = 3$. Equation (5.8) is applicable for low pH ($pH < pH_{ul}$), and high pH regimes $I_{pH} \cong 1$, (i.e.,$pH \geq pH_{ul}$), while Equations (5.7), (5.9) and (5.10) are applicable for both low and high pH regimes. Equation (5.9) applied by **Yoon-Sun et al.** [181] is based on the analogy of the **Andrews (1968)** model, Table 3. Where $K_{s,[H^+]}$ is the $[H^+]$ saturation constant and $K_{I,[H^+]}$ is the $[H^+]$ inhibition constant. The **Hill** function, Equation (5.10) is a non-competitive inhibition factor deduced via Equation (5.2), with $[H^+]^{\varphi} = \mathbb{I}$, $K_{pH}^{\varphi} = K_{I,j}$, and η, is a fitting constant unique to the system. This model is unpopular due to its steep variation in calculated pH inhibition [22].

As an evaluatory contribution, the substrate and product inhibition effects can be assumed to be accounted for by pH inhibition since the AD pH is mainly influenced by substrate and product composition [108,155,182]. However, this idea might be limited in processes with competitive substrate inhibition.

5.2. Influences of temperature on microbial activity

Unlike the pH inhibition approach, temperature dependence in microbial specific growth rate, μ is quite different, as reported by **Chezeau & Vial** [22] for μ_{max}. Equations (5.11) - (5.14) illustrate the dependency of μ_{max} on temperature. In the Arrhenius model, Equation (5.11), A, is the Arrhenius preexponential factor, R, the ideal gas constant, $\mathcal{E}$, the activation energy and T, the AD temperature. The Ratkowsky model, Equation (5.12), $\mathbb{A}$(K^{-1}·time^{-1}) and $\mathcal{B}$(K^{-1}) are constants, while T_{min} and T_{max} are the minimum and maximum temperature (K) at which the reaction rate is zero. Also available is

the Hinshelwood model, a combination of two Arrhenius models, Equation (5.13). Where the first and second part of this model describe the increase and decrease of microbial activity (within certain temperature limits). **Hashimoto et al.**[183] considered a model for methanogens, $\mu_{max,m}$ and acidogenes, $\mu_{max,a}$ based on linear relationship with temperature (℃), Equation (5.14) [11]. Comprehensive details on microbial activity dependence on temperature were reported by **Zwietering et al.** [180].

$$\mu_{max} = \mathbb{A}exp(-\mathcal{E}/RT) \quad (5.11)$$

$$\mu_{max} = \{\mathbb{A}(T - T_{min})\}^2 \{1 - exp[\mathcal{B}(T - T_{max})]\}^2 \quad (5.12)$$

$$\mu_{max} = \mathbb{A}_1 exp(-\mathcal{E}_1/RT) - \mathbb{A}_2 exp(-\mathcal{E}_2/RT) \quad (5.13)$$

$$\mu_{max,m} = \mu_{max,a} = 0.013T - 0.129 \quad (5.14)$$

5.3. Microbial death kinetics

In addition to microbial specific growth rate, μ, death rate, K_d is also applied to the microbe balance to prevent the overestimation of cell viability. K_d is dependent on factors like temperature, final product, and substrate [184] as indicated by Equations (5.15) - (5.17). Where K_{mB} (time $^{-1}$) and $Y_{B/S}$ are the maintenance coefficient, and the maximum yield of microbes on substrates.

$$K_d = \mathbb{A}exp(-E_a/RT) \quad (5.15)$$

$$K_d = \mathbb{A}exp(\mathcal{B}P) \quad (5.16)$$

$$K_d = K_{mB}Y_{B/S} \quad (5.17)$$

The decay coefficient (K_d) is usually about 5% of μ_{max}. It is common to ignore decay in methanogen growth, due to its low decay coefficient (about 1% of μ_{max}) [185].

5.4. Theoretical estimate of microbial and biogas yield

Microbes and biogas theoretical yield estimation for a given substrate (with known carbon, hydrogen, and oxygen composition) is essential to have an idea of their maximum possible AD yield. This estimation assumes the complete conversion of the substrate into CO_2 and CH_4. This enables comparisons between the theoretical and the experimental yields (by bottle assays) [24]. It can also be used to estimate $R_{\mathbb{J}}$, Equation (4.2), in the absence of experimental data. The generic expressional statement for transformation of organic matter in AD is given by Equation (5.18) [186].

Organic matter + H_2O + Nutrients = Microbes + Resistant organic matter + CO_2 + CH_4 + NH_3 + H_2S + Heat (5.18)

5.4.1. Determination of theoretical microbes' yield

According to Equation (5.18), not all organic matter is biodegradable, due to the presence of non-degradable components, inhibitory substances, operating conditions, etc. **Filer et al.**[53] reported that 10% of the substrate in AD is converted into microbes and transformed into heat and that following the VD1 4630 guideline - when cellulose is digested in a BMP test it produces a biogas yield of at least 80-85% of its theoretical maximum

The microbe yield, Y_{B/S_j} from a generic substrate, $C_{\mathbb{a}}H_{\mathbb{b}}O_{\mathbb{c}}N_{\mathbb{d}}$ can be deduced from Equation (5.19), on the basis that the chemical composition of microbes consist of 92% $C_5H_7O_2N$ on total dry weight [39].

$$C_{\mathbb{a}}H_{\mathbb{b}}O_{\mathbb{c}}N_{\mathbb{d}} + \left(\frac{\mathbb{a}}{5} - d\right)NH_3 \rightarrow \left(\frac{\mathbb{a}}{5}\right)C_5H_7O_2N + \left(\mathbb{c} - \frac{2\mathbb{a}}{5}\right)H_20 + \left(\frac{\mathbb{b} - 2\mathbb{c} - 3\mathbb{d}}{2}\right)H_2 \quad (5.19)$$

5.4.2. Determination of theoretical biogas yield

The theoretical biogas (CH_4 and CO_2) yield, Y_{G/S_j} can be estimated via diverse approaches. The **Buswell & Neave (1930)** stoichiometric balance is a typical example, based on the generic substrate, $C_{\mathbb{a}}H_{\mathbb{b}}O_{\mathbb{c}}N_{\mathbb{d}}$ [186],as given by Equations (5.20) and (5.21) or (5.22). Where M_j and $\mathbb{m}_j$ are the molar mass (i.e., 12) and stoichiometric ratio (i.e., $\mathbb{a}$) of carbon in the specific biogas species.

$$C_{\mathbb{a}}H_{\mathbb{b}}O_{\mathbb{c}}N_{\mathbb{d}} + \left(\frac{4\mathbb{a} - \mathbb{b} - 2\mathbb{c} + 3\mathbb{d}}{8}\right)H_2O \rightarrow \left(\frac{4a + \mathbb{b} - 2\mathbb{c} - 3\mathbb{d}}{8}\right)CH_4 + \left(\frac{4a - \mathbb{b} + 2\mathbb{c} + 3\mathbb{d}}{8}\right)CO_2 + \mathbb{d}NH_3 \quad (5.20)$$

$$Y_{G_j/S_j}(kg/kg) = \frac{M_j n_j}{(12\mathbb{a} + \mathbb{b} + 16\mathbb{c} + 14\mathbb{d})} \quad (5.21)$$

$$Y_{G_j/S_j}(m^3/kg) = \frac{23.415 n_j}{(12\mathbb{a} + \mathbb{b} + 16\mathbb{c} + 14\mathbb{d})} \quad (5.22)$$

6. Hydrolysis in anaerobic digestion

In literature reports on AD, contemplations exist on whether hydrolysis or methanogenesis is the rate-limiting step. For example, **Pavlostathis & Giraldo-Gomez** [187] suggested the feedstock hydrolysis step as the rate-limiting step. Therefore, it is important to elaborate and develop a model for the hydrolysis step. Hydrolysis rate is dependent on feedstock, F characteristics e.g., its states (liquid or solid), solubility, etc. Hydrolysis models can be either first-order kinetic or mechanistic based (i.e., surface-based, and growth-based) models [188].

6.1. First-order kinetic model, FKM

The FKM assumes a linear relationship with feedstock mass, m_F, Equation (6.1). It was initially developed for particulate feedstocks, and therefore its rate and kinetic constant, K_{FH} is dependent on changes in particulate sizes [188,189]. When deducing K_{FH} all physical and biochemical mechanisms are lumped, hence not robust enough for simulation, and optimisation of the actual process. Despite said limitations - ADM1 [8], **Lopez et al.**[190], and **Luo et al.**[191] applied and found this model adequate.

$$dm_F/dt = -K_{FH}m_F \quad (6.1)$$

6.2. Surface-based model, SBM

This model assumes that particulate enzymes from microbe activity are present in higher amounts than feedstock particulates since such enzymes are attached to all available feedstock surfaces and that the amount of feedstock particles remains constant during hydrolysis [188]. The rate of change of feedstock dF/dt, is therefore dependent on available feedstock surface, $\Gamma(cm^2)$, and kinetic constant, K_{FS} ($g \cdot cm^{-2} \cdot time^{-1}$), Equation (6.2). The feedstock surface is assumed to peel layer by layer, Fig. 6a hence the SBM is also called the shrinking core model. **Sanders et al.**[192] found the SBM good for hydrolysis in AD.

$$dF/dt = -K_{FS}\Gamma \quad (6.2)$$

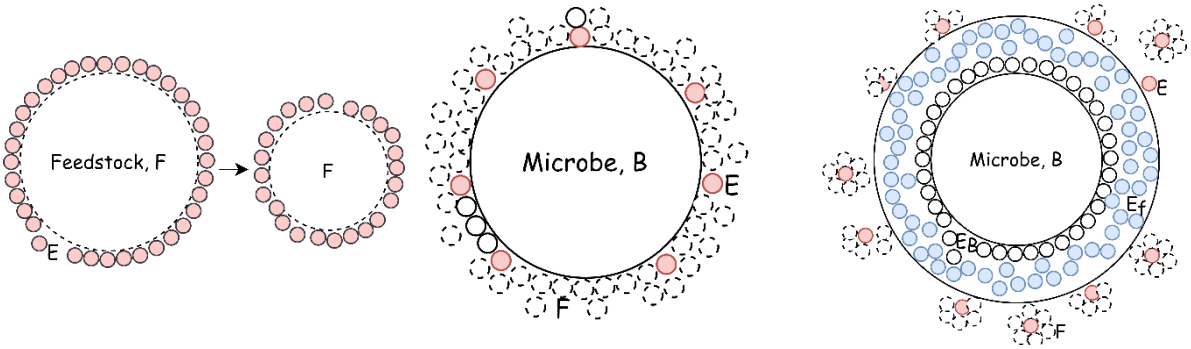
6.3. Growth-based model, GBM

This model applies to soluble feedstocks, as such, it is assumed that the feedstock area is infinite, and enzymes are assumed deficient; hence microbial activity is the hydrolysis rate-limiting factor [188]. The model is similar to the Michaelis-Menten kinetic, Equations (6.3) - (6.4), and resembles the Contois model [189,193–195]. Where K_E is the enzymatic rate constant ($time^{-1}$), K_M, the half velocity constant ($g \cdot L^{-1}$), and B & E, microbes & enzymes concentration ($g \cdot L^{-1}$). Analysis of Equation (6.3) implies that it is a multistep model since steps for the synthesis of microbes/enzymes like Equation (4.1), diffusion and adsorption of enzymes into particulates need to be modelled. **Vavilin et al.**[194]

and **Veluchamy & Kalamdhad** [196] assumed that microbes attach to feedstock particles, produce enzymes in their vicinity and benefit from soluble products released. While **Jain et al.**[27] assumed microbes secrete enzymes (on their surface, E_B and film around the microbe, E_f) and diffuse to the bulk liquid (i.e. E) where they are adsorbed onto or react with soluble feedstock. Analysis of these works indicates that the model is robust, especially for investigating whether the extracellular enzyme catalysed hydrolysis is the rate-limiting step in AD.

$$B \rightarrow E, E + F \rightleftharpoons EF \Rightarrow E + S \quad (6.3)$$

$$dF/dt = -K_E E\, F/(K_M + F) \quad (6.4)$$



(a) Shrinking core model (b) Growth-based model [194] (c) Growth-based model [27]

Fig. 6. Mechanism of feedstock hydrolysis in anaerobic digestion; E – enzyme, E_B – enzymes on microbes surface, E_f – enzymes in the film around the microbe

In summary, FKM and SBM are simplified and may not be adequate to investigate the rate-limiting step in AD, unlike GBM. However, attempts have been made to improve them, via: Incorporation of the non-degradable fraction, θ and the shape factor, σ of the feedstock (σ is 2/3, 1/2 and 0 for spherical, cylindrical, and plate-form particles) to the FKM, which may result to nth-kinetic [25,193,194]; Incorporation of the FKM into SBM by considering hydrolysis a function of the area-mass ratio and concentration of feedstock [197]; and consideration of a two-phase model that incorporates microbes kinetic into the FKM, and simultaneously consider microbes growth model like, Equation (4.1) [190,194,198].

7. Conclusion

To enhance the comparison of results from biogas models, a systematic approach has been established to classify biogas models into: **single-equation models** (analytical and multi-regression, which can be a cumulative or dynamic model) or **multi-step dynamic models** (SSDM, TSDM or MSDM). Most **single-equation models** are simple, requiring limited numbers and inexpensive experiments to curve fit, and subsequently can be easily used for simulation and control purposes. Although they are not as accurate compared to the **multi-step dynamic models**, the resulting data (e.g., biogas production potential, maximum biogas production rate) are useful, and as such suitable for AD preliminary studies. In contrast, **multi-step dynamic models** are complex and accurate but require substantial number of input data and expensive experiments to be developed. Depending on their complexity they are difficult to solve and apply to control purposes - especially in the order of MSDM >TSDM > SSDM. The magnitude of the difference in accuracy between these models is dependent on the degree of AD sensitivity to the intermediates produced.

In addition, related phenomena like microbial kinetics, pH estimation or feedstock hydrolysis and their corresponding models essential for developing and implementing multi-step dynamic models were discussed. Since biochemical processes involved in AD are dependent on pH and temperature, these process conditions and their dynamics are important aspects in AD modelling. Note that these parameters are also important for monitoring of the AD stability and estimation of thermochemical properties. Deducing the pH dynamics was found to be appropriately implemented when the evolution of biogas from the dissolved liquid phase to gas headspace was considered. This is because it makes possible the deduction of dynamics for unevolved and partial pressures of evolved biogas species (especially CO_2 and H_2) vital for controlling AD pressure and stability. Another notable observation is that water vapour contributes to the total system pressure which highlights the need to consider dynamics for consumption, formation, and evaporation of water in AD. Interestingly, this phenomenon has not been considered in most literature, similarly as the impact of temperature. Finally, the possibility of inhomogeneity of concentration and AD temperature within the bioreactor substantiated the need to model and discuss the effect of stirring operation. Consequently, further research in AD modelling should consider the effect of stirring.

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References

[1] Ritchie H, Roser M. Renewable Energy. Our World Data 2020.

[2] Ng'andwe P, Ratnasingam J, Mwitwa J, Tembo JC. Wood and Wood Products, Markets and Trade. For. Policy, Econ. Mark. Zambia, Elsevier Inc.; 2015, p. 27–66. https://doi.org/10.1016/B978-0-12-804090-4.00002-1.

[3] World Bank Group. Renewable energy consumption. World Bank 2021. https://data.worldbank.org (accessed April 10, 2021).

[4] Lobo MG, Dorta E. Utilization and Management of Horticultural Waste. Postharvest Technol. Perish. Hortic. Commod., Elsevier; 2019, p. 639–66. https://doi.org/10.1016/B978-0-12-813276-0.00019-5.

[5] Fedailaine M, Moussi K, Khitous M, Abada S, Saber M, Tirichine N. Modeling of the anaerobic digestion of organic waste for biogas production. Procedia Comput. Sci., vol. 52, Elsevier B.V.; 2015, p. 730–7. https://doi.org/10.1016/j.procs.2015.05.086.

[6] Wade MJ. Not just numbers: Mathematical modelling and its contribution to anaerobic digestion processes. Processes 2020;8:888. https://doi.org/10.3390/PR8080888.

[7] Van Hulle SWH, Vesvikar M, Poutiainen H, Nopens I. Importance of scale and hydrodynamics for modeling anaerobic digester performance. Chem Eng J 2014;255:71–7. https://doi.org/10.1016/j.cej.2014.06.041.

[8] Batstone DJ, Keller J, Angelidaki I, Kalyuzhnyi S V., Pavlostathis SG, Rozzi A, et al. The IWA Anaerobic Digestion Model No 1 (ADM1). Water Sci Technol 2002;45:65–73. https://doi.org/10.2166/wst.2002.0292.

[9] Nielfa A, Cano R, Fdz-Polanco M. Theoretical methane production generated by the co-

digestion of organic fraction municipal solid waste and biological sludge. Biotechnol Reports 2015;5:14–21. https://doi.org/10.1016/j.btre.2014.10.005.

[10] Jiunn-Jyi L, Yu-You L, Noike T. Influences of pH and moisture content on the methane production in high-solids sludge digestion. Water Res 1997;31:1518–24. https://doi.org/10.1016/S0043-1354(96)00413-7.

[11] Hill DT, Barth CL. A Dynamic Model for Simulation of Animal Waste Digestion. Water Pollut Control Fed 1977;49:2129–43.

[12] Havlík I, Votruba J, Sobotka M. Mathematical modelling of the anaerobic digestion process: Application of dynamic mass-energy balance. Folia Microbiol (Praha) 1986;31:56–68. https://doi.org/10.1007/BF02928680.

[13] Yu L, Wensel PC. Mathematical Modeling in Anaerobic Digestion (AD). J Bioremediation Biodegrad 2013;s4. https://doi.org/10.4172/2155-6199.s4-003.

[14] Ramachandran A, Rustum R, Adeloye AJ. Review of anaerobic digestion modeling and optimization using nature-inspired techniques. Processes 2019;7:953. https://doi.org/10.3390/PR7120953.

[15] Velázquez-Martí B, W. Meneses-Quelal O, Gaibor-Chavez J, Niño-Ruiz Z. Review of Mathematical Models for the Anaerobic Digestion Process. Anaerob. Dig., IntechOpen; 2019. https://doi.org/10.5772/intechopen.80815.

[16] Kythreotou N, Florides G, Tassou SA. A review of simple to scientific models for anaerobic digestion. Renew Energy 2014;71:701–14. https://doi.org/10.1016/j.renene.2014.05.055.

[17] Gerber M, Span R. An analysis of available mathematical models for anaerobic digestion of organic substances for production of biogas. Int. gas union Res. Conf. , Paris: 2008, p. 1–30.

[18] Weinrich S, Nelles M. Systematic simplification of the Anaerobic Digestion Model No. 1 (ADM1) – Model development and stoichiometric analysis. Bioresour Technol 2021;333:125124. https://doi.org/10.1016/J.BIORTECH.2021.125124.

[19] Manchala KR, Sun Y, Zhang D, Wang Z-W. Anaerobic Digestion Modelling, 2017, p. 69–141. https://doi.org/10.1016/bs.aibe.2017.01.001.

[20] Simeonov I, Stoyanov S. Modelling and Dynamic Compensator Control of the Anaerobic Digestion of Organic Wastes. Chem Biochem Eng Q 2003;17:285–92.

[21] Beuvink JM, Kogut J. Modeling gas production kinetics of grass silages incubated with buffered ruminal fluid. J Anim Sci 1993;71:1041–6. https://doi.org/10.2527/1993.7141041x.

[22] Chezeau B, Vial C. Modeling and Simulation of the Biohydrogen Production Processes. Biohydrogen, Elsevier; 2019, p. 445–83. https://doi.org/10.1016/b978-0-444-64203-5.00019-8.

[23] Ma J, Frear C, Wang ZW, Yu L, Zhao Q, Li X, et al. A simple methodology for rate-limiting step determination for anaerobic digestion of complex substrates and effect of microbial community ratio. Bioresour Technol 2013;134:391–5. https://doi.org/10.1016/j.biortech.2013.02.014.

[24] Meegoda JN, Li B, Patel K, Wang LB. A review of the processes, parameters, and optimization of anaerobic digestion. Int J Environ Res Public Health 2018;15:2224. https://doi.org/10.3390/ijerph15102224.

[25] Yang G, Sun Y, Li L, Lv P, Kong X, Huang D. Hydrolysis dynamics for batch anaerobic digestion of elephant grass. RSC Adv 2018;8:22670–5. https://doi.org/10.1039/c8ra01115j.

[26] Van Haandel AC, Monroy O, Rustrian E, Cervantes FJ. Principles of process design for industrial wastewater treatment systems. In: Cervantes FJ, Pavlostathis SG, Van Haande AC,

editors. Adv. Biol. Treat. Process. Ind. Wastewaters - Princ. Appl. , London: IWA Publishing; 2006, p. 47–140.

[27] Jain S, Lala AK, Bhatia SK, Kudchadker AP. Modelling of hydrolysis controlled anaerobic digestion. J Chem Technol Biotechnol 1992;53:337–44. https://doi.org/10.1002/jctb.280530404.

[28] Maleki E, Bokhary A, Liao BQ. A review of anaerobic digestion bio-kinetics. Rev Environ Sci Biotechnol 2018;17:691–705. https://doi.org/10.1007/s11157-018-9484-z.

[29] Uçkun Kiran E, Stamatelatou K, Antonopoulou G, Lyberatos G. Production of biogas via anaerobic digestion. Handb. Biofuels Prod. Process. Technol. Second Ed., Elsevier Inc.; 2016, p. 259–301. https://doi.org/10.1016/B978-0-08-100455-5.00010-2.

[30] Polman EMN, Gruter GJM, Parsons JR, Tietema A. Comparison of the aerobic biodegradation of biopolymers and the corresponding bioplastics: A review. Sci Total Environ 2021;753:141953. https://doi.org/10.1016/j.scitotenv.2020.141953.

[31] Raveendran S, Parameswaran B, Ummalyma SB, Abraham A, Mathew AK, Madhavan A, et al. Applications of microbial enzymes in food industry. Food Technol Biotechnol 2018;56:16–30. https://doi.org/10.17113/ftb.56.01.18.5491.

[32] Mazzucotelli CA, Ponce AG, Kotlar CE, Moreira M del R. Isolation and characterization of bacterial strains with a hydrolytic profile with potential use in bioconversion of agroindustial by-products and waste. Food Sci Technol 2013;33:295–303. https://doi.org/10.1590/S0101-20612013005000038.

[33] Gerardi MH. The Microbiology of Anaerobic Digesters. Hoboken, NJ, USA: John Wiley & Sons, Inc.; 2003. https://doi.org/10.1002/0471468967.

[34] Shin J Du, Xu C, Kim SH, Kim H, Mahmood N, Kim M. Biomass Conversion of Plant Residues. Food Bioconversion, vol. 2, Elsevier; 2017, p. 351–83. https://doi.org/10.1016/B978-0-12-811413-1.00010-3.

[35] Shah YT. Chemical energy from natural and synthetic gas. CRC Press; 2017. https://doi.org/10.1201/9781315302355.

[36] Manyi-Loh CE, Mamphweli SN, Meyer EL, Okoh AI, Makaka G, Simon M. Microbial anaerobic digestion (bio-digesters) as an approach to the decontamination of animal wastes in pollution control and the generation of renewable energy. Int J Environ Res Public Health 2013;10:4390–417. https://doi.org/10.3390/ijerph10094390.

[37] Ali Shah F, Mahmood Q, Maroof Shah M, Pervez A, Ahmad Asad S. Microbial ecology of anaerobic digesters: The key players of anaerobiosis. Sci World J 2014;2014:1–21. https://doi.org/10.1155/2014/183752.

[38] Zhang J, Wang S, Wang Y. Biobutanol Production From Renewable Resources, 2016, p. 1–68. https://doi.org/10.1016/bs.aibe.2016.09.001.

[39] Moletta R, Verrier D, Albagnac G. Dynamic modelling of anaerobic digestion. Water Res 1986;20:427–34. https://doi.org/10.1016/0043-1354(86)90189-2.

[40] Silva OB da, Carvalho LS, Almeida GC da, Oliveira JD de, Carmo TS, Parachin NS. Biogas - Turning Waste into Clean Energy. Ferment. Process., InTech; 2017. https://doi.org/10.5772/64262.

[41] Ramos-Suárez JL, Carreras Arroyo N, González-Fernández C. Organic Waste Treatment, and Nutrient Loop Closure. In: Singh B, Bauddh K, Bux F, editors. Algae Environ. Sustain., vol. 7. 1st ed., Springer India; 2015, p. 1–8. https://doi.org/10.1007/978-81-322-2641-3_1.

[42] Anderson K, Sallis P, Uyanik S. Anaerobic treatment processes. Handb. Water Wastewater

Microbiol., Elsevier Inc.; 2003, p. 391–426. https://doi.org/10.1016/B978-012470100-7/50025-X.

[43] Serrano-Silva N, Sarria-Guzmán Y, Dendooven L, Luna-Guido M. Methanogenesis and Methanotrophy in Soil: A Review. Pedosphere 2014;24:291–307. https://doi.org/10.1016/S1002-0160(14)60016-3.

[44] Nguyen D, Nitayavardhana S, Sawatdeenarunat C, Surendra KC, Khanal SK. Biogas production by anaerobic digestion: Status and perspectives. Biomass, Biofuels, Biochem. Biofuels Altern. Feed. Convers. Process. Prod. Liq. Gaseous Biofuels, Elsevier; 2019, p. 763–78. https://doi.org/10.1016/B978-0-12-816856-1.00031-2.

[45] Abbassi-Guendouz A, Trably E, Hamelin J, Dumas C, Steyer JP, Delgenès JP, et al. Microbial community signature of high-solid content methanogenic ecosystems. Bioresour Technol 2013;133:256–62. https://doi.org/10.1016/j.biortech.2013.01.121.

[46] Hornung A. Transformation of Biomass: Theory to Practice. Chichester, UK: Wiley Blackwell; 2014. https://doi.org/10.1002/9781118693643.

[47] Nges IA, Liu J. Effects of solid retention time on anaerobic digestion of dewatered-sewage sludge in mesophilic and thermophilic conditions. Renew Energy 2010;35:2200–6. https://doi.org/10.1016/j.renene.2010.02.022.

[48] Bolzonella D, Pavan P, Battistoni P, Cecchi F. Mesophilic anaerobic digestion of waste activated sludge: Influence of the solid retention time in the wastewater treatment process. Process Biochem 2005;40:1453–60. https://doi.org/10.1016/j.procbio.2004.06.036.

[49] Rizvi H, Ahmad N, Abbas F, Bukhari IH, Yasar A, Ali S, et al. Start-up of UASB reactors treating municipal wastewater and effect of temperature/sludge age and hydraulic retention time (HRT) on its performance. Arab J Chem 2015;8:780–6. https://doi.org/10.1016/j.arabjc.2013.12.016.

[50] Lindmark J, Thorin E, Bel Fdhila R, Dahlquist E. Effects of mixing on the result of anaerobic digestion: Review. Renew Sustain Energy Rev 2014;40:1030–47. https://doi.org/10.1016/j.rser.2014.07.182.

[51] Singh B, Szamosi Z, Siménfalvi Z. Impact of mixing intensity and duration on biogas production in an anaerobic digester: a review. Crit Rev Biotechnol 2020;40:508–21. https://doi.org/10.1080/07388551.2020.1731413.

[52] Drosg B, Braun R, Bochmann G, Al Saedi T. Analysis and characterisation of biogas feedstocks. Biogas Handb. Sci. Prod. Appl., Elsevier Inc.; 2013, p. 52–84. https://doi.org/10.1533/9780857097415.1.52.

[53] Filer J, Ding HH, Chang S. Biochemical methane potential (BMP) assay method for anaerobic digestion research. Water (Switzerland) 2019;11:921. https://doi.org/10.3390/w11050921.

[54] Barampouti EMP, Mai ST, Vlyssides AG. Dynamic modeling of biogas production in an UASB reactor for potato processing wastewater treatment. Chem Eng J 2005;106:53–8. https://doi.org/10.1016/j.cej.2004.06.010.

[55] Das A, Mondal C. Comparative Kinetic Study of Anaerobic Treatment of Thermally Pretreated Source-Sorted Organic Market Refuse. J Eng (United Kingdom) 2015;2015:1–14. https://doi.org/10.1155/2015/684749.

[56] Lo HM, Kurniawan TA, Sillanpää MET, Pai TY, Chiang CF, Chao KP, et al. Modeling biogas production from organic fraction of MSW co-digested with MSWI ashes in anaerobic bioreactors. Bioresour Technol 2010;101:6329–35. https://doi.org/10.1016/j.biortech.2010.03.048.

[57] Shitophyta LM, Maryudi. Comparison of kinetic model for biogas production from corn cob. IOP Conf. Ser. Mater. Sci. Eng., vol. 345, Institute of Physics Publishing; 2018, p. 012004. https://doi.org/10.1088/1757-899X/345/1/012004.

[58] Ejimofor MI, Ezemagu IG, Menkiti MC. Biogas production using coagulation sludge obtained from paint wastewater decontamination: Characterization and anaerobic digestion kinetics". Curr Res Green Sustain Chem 2020;3:100024. https://doi.org/10.1016/j.crgsc.2020.100024.

[59] Kovács Veszelovszki P, Keszthelyi-Szabó G, Szendrő P. Enhancing Biogas Production Kinetic of Meat Industrialwastewater by Microwave Pretreatment. Hungarian Agric Eng 2018:44–8. https://doi.org/10.17676/hae.2018.34.44.

[60] Ravindra P, Yong KY, Veera Rao VPR. Production of biogas from palm oil mill effluent. Adv. Bioprocess Technol., Cham: Springer International Publishing; 2015, p. 99–112. https://doi.org/10.1007/978-3-319-17915-5_6.

[61] Ahmed S, Kazda M. Characteristics of on-demand biogas production by using sugar beet silage. Anaerobe 2017;46:114–21. https://doi.org/10.1016/j.anaerobe.2017.04.016.

[62] Das Ghatak M, Mahanta P. Comparison of kinetic models for biogas production rate from saw dust. IJRET Int J Res Eng Technol 2014;3:2321–7308.

[63] Howell G, Bennett C, Materić D. A comparison of methods for early prediction of anaerobic biogas potential on biologically treated municipal solid waste. J Environ Manage 2019;232:887–94. https://doi.org/10.1016/j.jenvman.2018.11.137.

[64] Siripatana C, Jijai S, O-Thong S, Ismail N. Modeling of Biomethane Production from Agro-Industrial Wastewaters with Constant Biomass: Analysis of Gompertz Equation. Int. Conf. Environ. Res. Technol., School of Industrial Technology, Universiti Sains Malaysia; 2015, p. 1–6.

[65] Zuru AA, Dangoggo SM, Birnin-Yauri UA, Tambuwal AD. Adoption of thermogravimetric kinetic models for kinetic analysis of biogas production. Renew Energy 2004;29:97–107. https://doi.org/10.1016/S0960-1481(03)00074-0.

[66] Pramanik SK, Suja FB, Porhemmat M, Pramanik BK. Performance and kinetic model of a single-stage anaerobic digestion system operated at different successive operating stages for the treatment of food waste. Processes 2019;7:600. https://doi.org/10.3390/pr7090600.

[67] Bilgili MS, Demir A, Varank G. Evaluation and modeling of biochemical methane potential (BMP) of landfilled solid waste: A pilot scale study. Bioresour Technol 2009;100:4976–80. https://doi.org/10.1016/j.biortech.2009.05.012.

[68] De Gioannis G, Muntoni A, Cappai G, Milia S. Landfill gas generation after mechanical biological treatment of municipal solid waste. Estimation of gas generation rate constants. Waste Manag 2009;29:1026–34. https://doi.org/10.1016/j.wasman.2008.08.016.

[69] Córdoba V, Fernández M, Santalla E. The effect of substrate/inoculum ratio on the kinetics of methane production in swine wastewater anaerobic digestion. Environ Sci Pollut Res 2018;25:21308–17. https://doi.org/10.1007/s11356-017-0039-6.

[70] Schofield P, Pitt RE, Pell AN. Kinetics of fiber digestion from in vitro gas production. J Anim Sci 1994;72:2980–91. https://doi.org/10.2527/1994.72112980x.

[71] Lay J-J, Li Y-Y, Noike T. Effect of Moisture Content and Chemical Nature on Methane Fermentation Characteristics of Municipal Solid Wastes. Doboku Gakkai Ronbunshu 1996:101–8. https://doi.org/10.2208/jscej.1996.552_101.

[72] Pham Van D, Hoang Minh G, Pham Phu ST, Fujiwara T. A new kinetic model for biogas production from co-digestion by batch mode. Glob J Environ Sci Manag 2018;4:251–62.

https://doi.org/10.22034/GJESM.2018.03.001.

[73] Achinas S, Krooneman J, Euverink GJW. Enhanced Biogas Production from the Anaerobic Batch Treatment of Banana Peels. Engineering 2019;5:970–8. https://doi.org/10.1016/j.eng.2018.11.036.

[74] Zahan Z, Othman MZ, Muster TH. Anaerobic digestion/co-digestion kinetic potentials of different agro-industrial wastes: A comparative batch study for C/N optimisation. Waste Manag 2018;71:663–74. https://doi.org/10.1016/j.wasman.2017.08.014.

[75] Deepanraj B, Sivasubramanian V, Jayaraj S. Effect of substrate pretreatment on biogas production through anaerobic digestion of food waste. Int J Hydrogen Energy 2017;42:26522–8. https://doi.org/10.1016/j.ijhydene.2017.06.178.

[76] Zwietering MH, Jongenburger I, Rombouts FM, van 't Riet K. Modeling of the Bacterial Growth Curve. Appl Environ Microbiol 1990;56:1875–81. https://doi.org/10.1128/aem.56.6.

[77] Alizadeh HHA, Seifi R, Radmard SA. Evaluation of the anaerobic digestion of kitchen waste by thermal pretreatment in a batch leach bed reactor with down flow and the kinetics of methane yields. Biofuels 2018;9:315–23. https://doi.org/10.1080/17597269.2016.1266235.

[78] Ware A, Power N. Modelling methane production kinetics of complex poultry slaughterhouse wastes using sigmoidal growth functions. Renew Energy 2017;104:50–9. https://doi.org/10.1016/j.renene.2016.11.045.

[79] Zhang H, An D, Cao Y, Tian Y, He J. Modeling the Methane Production Kinetics of Anaerobic Co-Digestion of Agricultural Wastes Using Sigmoidal Functions. Energies 2021, Vol 14, Page 258 2021;14:258. https://doi.org/10.3390/EN14020258.

[80] Pererva Y, Miller CD, Sims RC. Existing Empirical Kinetic Models in Biochemical Methane Potential (BMP) Testing, Their Selection and Numerical Solution. Water 2020, Vol 12, Page 1831 2020;12:1831. https://doi.org/10.3390/W12061831.

[81] Li L, Kong X, Yang F, Li D, Yuan Z, Sun Y. Biogas production potential and kinetics of microwave and conventional thermal pretreatment of grass. Appl Biochem Biotechnol 2012;166:1183–91. https://doi.org/10.1007/s12010-011-9503-9.

[82] Pitt RE, Cross TL, Pell AN, Schofield P, Doane PH. Use of in vitro gas production models in ruminal kinetics. Math Biosci 1999;159:145–63. https://doi.org/10.1016/S0025-5564(99)00020-6.

[83] Shen J, Yan H, Zhang R, Liu G, Chen C. Characterization and methane production of different nut residue wastes in anaerobic digestion. Renew Energy 2018;116:835–41. https://doi.org/10.1016/j.renene.2017.09.018.

[84] Schenute J. A versatile growth model with statistically stable parameters. Can J Fish Aquat Sci 1981;38:1128–40. https://doi.org/10.1139/f81-153.

[85] Ramprakash B, Muthukumar K. Influence of sulfuric acid concentration on biohydrogen production from rice mill wastewater using pure and coculture of Enterobacter aerogenes and Citrobacter freundii. Int J Hydrogen Energy 2018;43:9254–8. https://doi.org/10.1016/j.ijhydene.2018.03.198.

[86] Bentil DE, Osei BM, Ellingwood CD, Hoffmann JP. Analysis of a Schnute postulate-based unified growth model for model selection in evolutionary computations. BioSystems 2007;90:467–74. https://doi.org/10.1016/j.biosystems.2006.11.006.

[87] Donoso-Bravo A, Pérez-Elvira SI, Fdz-Polanco F. Application of simplified models for anaerobic biodegradability tests. Evaluation of pre-treatment processes. Chem Eng J 2010;160:607–14. https://doi.org/10.1016/j.cej.2010.03.082.

[88] El-Mashad HM. Kinetics of methane production from the codigestion of switchgrass and Spirulina platensis algae. Bioresour Technol 2013;132:305–12. https://doi.org/10.1016/j.biortech.2012.12.183.

[89] Syaichurrozi I. Biogas production from co-digestion Salvinia molesta and rice straw and kinetics. Renew Energy 2018;115:76–86. https://doi.org/10.1016/j.renene.2017.08.023.

[90] Parralejo AI, Royano L, González J, González JF. Small scale biogas production with animal excrement and agricultural residues. Ind Crops Prod 2019;131:307–14. https://doi.org/10.1016/j.indcrop.2019.01.059.

[91] Guan R, Gu J, Wachemo AC, Yuan H, Li X. Novel Insights into Anaerobic Digestion of Rice Straw Using Combined Pretreatment with CaO and the Liquid Fraction of Digestate: Anaerobic Digestion Performance and Kinetic Analysis. Energy and Fuels 2020;34:1119–30. https://doi.org/10.1021/acs.energyfuels.9b02104.

[92] Coelho MMH, Morais NWS, Ferreira TJT, Silva FSS, Pereira EL, dos Santos AB. Carboxylic acids production using residual glycerol as a substrate in anaerobic fermentation: A kinetic modeling study. Biomass and Bioenergy 2020;143:105874. https://doi.org/10.1016/j.biombioe.2020.105874.

[93] Tian Y, Yang K, Zheng L, Han X, Xu Y, Li Y, et al. Modelling Biogas Production Kinetics of Various Heavy Metals Exposed Anaerobic Fermentation Process Using Sigmoidal Growth Functions. Waste and Biomass Valorization 2020;11:4837–48. https://doi.org/10.1007/s12649-019-00810-x.

[94] Cao W, Sun C, Li X, Qiu J, Liu R. Methane production enhancement from products of alkaline hydrogen peroxide pretreated sweet sorghum bagasse. RSC Adv 2017;7:5701–7. https://doi.org/10.1039/c6ra25798d.

[95] Zhao C, Yan H, Liu Y, Huang Y, Zhang R, Chen C, et al. Bio-energy conversion performance, biodegradability, and kinetic analysis of different fruit residues during discontinuous anaerobic digestion. Waste Manag 2016;52:295–301. https://doi.org/10.1016/j.wasman.2016.03.028.

[96] Kainthola J, Kalamdhad AS, Goud V V., Goel R. Fungal pretreatment and associated kinetics of rice straw hydrolysis to accelerate methane yield from anaerobic digestion. Bioresour Technol 2019;286:121368. https://doi.org/10.1016/j.biortech.2019.121368.

[97] Veluchamy C, Kalamdhad AS. Enhancement of hydrolysis of lignocellulose waste pulp and paper mill sludge through different heating processes on thermal pretreatment. J Clean Prod 2017;168:219–26. https://doi.org/10.1016/j.jclepro.2017.09.040.

[98] Çetinkaya AY, Yetilmezsoy K. Evaluation of anaerobic biodegradability potential and comparative kinetics of different agro-industrial substrates using a new hybrid computational coding scheme. J Clean Prod 2019;238:117921. https://doi.org/10.1016/j.jclepro.2019.117921.

[99] Zaidi AA, RuiZhe F, Shi Y, Khan SZ, Mushtaq K. Nanoparticles augmentation on biogas yield from microalgal biomass anaerobic digestion. Int J Hydrogen Energy 2018;43:14202–13. https://doi.org/10.1016/j.ijhydene.2018.05.132.

[100] Zaidi AA, RuiZhe F, Malik A, Khan SZ, Bhutta AJ, Shi Y, et al. Conjoint effect of microwave irradiation and metal nanoparticles on biogas augmentation from anaerobic digestion of green algae. Int J Hydrogen Energy 2019;44:14661–70. https://doi.org/10.1016/j.ijhydene.2019.02.245.

[101] Motte JC, Escudié R, Bernet N, Delgenes JP, Steyer JP, Dumas C. Dynamic effect of total solid content, low substrate/inoculum ratio and particle size on solid-state anaerobic digestion. Bioresour Technol 2013;144:141–8. https://doi.org/10.1016/j.biortech.2013.06.057.

[102] Al-Wahaibi A, Osman AI, Al-Muhtaseb AH, Alqaisi O, Baawain M, Fawzy S, et al. Techno-

economic evaluation of biogas production from food waste via anaerobic digestion. Sci Reports 2020 101 2020;10:1–16. https://doi.org/10.1038/s41598-020-72897-5.

[103] Abu-Reesh IM. Kinetics of anaerobic digestion of labaneh whey in a batch reactor. African J Biotechnol 2014;13:1745–55. https://doi.org/10.5897/AJB2013.13310.

[104] Alfarjani F, Aboderheeba AKM, Benyounis K, Olabi A-G. Modelling Anaerobic Digestion Process for Grass Silage After Beating Treatment Using Design of Experiment. Causes, Impacts Solut. to Glob. Warm., New York, NY: Springer New York; 2013, p. 675–95. https://doi.org/10.1007/978-1-4614-7588-0_35.

[105] Mu Y, Yu HQ, Wang G. A kinetic approach to anaerobic hydrogen-producing process. Water Res 2007;41:1152–60. https://doi.org/10.1016/j.watres.2006.11.047.

[106] Chaib Draa K. Observation and control of anaerobic digestion processes for improved biogas production. Université de Lorraine ; Université du Luxembourg; 2017.

[107] Hassam S, Ficara E, Leva A, Harmand J. A generic and systematic procedure to derive a simplified model from the anaerobic digestion model No. 1 (ADM1). Biochem Eng J 2015;99:193–203. https://doi.org/10.1016/j.bej.2015.03.007.

[108] Kiely G, Tayfur G, Dolan C, Tanji K. Physical and mathematical modelling of anaerobic digestion of organic wastes. Water Res 1997;31:534–40. https://doi.org/10.1016/S0043-1354(96)00175-3.

[109] Haugen F, Bakke R, Lie B. Adapting Dynamic Mathematical Models to a Pilot Anaerobic Digestion Reactor. Model Identif Control A Nor Res Bull 2013;34:35–54. https://doi.org/10.4173/mic.2013.2.1.

[110] Saeed M, Fawzy S, El-Saadawi M. Modeling and simulation of biogas-fueled power system. Int J Green Energy 2019;16:125–51. https://doi.org/10.1080/15435075.2018.1549997.

[111] Ma J, Zhao QB, Laurens LLM, Jarvis EE, Nagle NJ, Chen S, et al. Mechanism, kinetics and microbiology of inhibition caused by long-chain fatty acids in anaerobic digestion of algal biomass. Biotechnol Biofuels 2015;8:141. https://doi.org/10.1186/s13068-015-0322-z.

[112] Flores-Estrella RA, Alcaraz-González V, García-Sandoval JP, González-Álvarez V. Robust output disturbance rejection control for anaerobic digestion processes. J Process Control 2019;75:15–23. https://doi.org/10.1016/j.jprocont.2018.12.012.

[113] Kil H, Li D, Xi Y, Li J. Model predictive control with on-line model identification for anaerobic digestion processes. Biochem Eng J 2017;128:63–75. https://doi.org/10.1016/j.bej.2017.08.004.

[114] Alcaraz-González V, Harmand J, Rapaport A, Steyer JP, González-Alvarez V, Pelayo-Ortiz C. Application of a robust interval observer to an anaerobic digestion process. Dev Chem Eng Miner Process 2005;13:267–78. https://doi.org/10.1002/apj.5500130308.

[115] Alcaraz-González V, Harmand J, Rapaport A, Steyer JP, González-Alvarez V, Pelayo-Ortiz C. Software sensors for highly uncertain WWTPs: A new approach based on interval observers. Water Res 2002;36:2515–24. https://doi.org/10.1016/S0043-1354(01)00466-3.

[116] Sari T, Benyahia B. The Operating Diagram for a Two-Step Anaerobic Digestion Model 2020.

[117] Boubaker F, Ridha BC. Modelling of the mesophilic anaerobic co-digestion of olive mill wastewater with olive mill solid waste using anaerobic digestion model No. 1 (ADM1). Bioresour Technol 2008;99:6565–77. https://doi.org/10.1016/j.biortech.2007.11.035.

[118] Bornhöft A, Hanke-Rauschenbach R, Sundmacher K. Steady-state analysis of the Anaerobic Digestion Model No. 1 (ADM1). Nonlinear Dyn 2013;73:535–49. https://doi.org/10.1007/s11071-013-0807-x.

[119] Beschkov V, Sapundzhiev T, Angelov I. Modelling of biogas production from glycerol by anaerobic process in a baffled multi-stage digestor. Biotechnol Biotechnol Equip 2012;26:3244–8. https://doi.org/10.5504/bbeq.2012.0061.

[120] Keshtkar A, Ghaforian H, Abolhamd G, Meyssami B. Dynamic simulation of cyclic batch anaerobic digestion of cattle manure. Bioresour Technol 2001;80:9–17. https://doi.org/10.1016/S0960-8524(01)00071-2.

[121] Balmant W, Oliveira BH, Mitchell DA, Vargas JVC, Ordonez JC. Optimal operating conditions for maximum biogas production in anaerobic bioreactors. Appl Therm Eng 2014;62:197–206. https://doi.org/10.1016/j.applthermaleng.2013.09.033.

[122] Bergland WH, Dinamarca C, Bakke R. Temperature Effects in Anaerobic Digestion Modeling. Proc 56th Conf Simul Model (SIMS 56), October, 7-9, 2015, Linköping Univ Sweden 2015;119:261–9. https://doi.org/10.3384/ecp15119261.

[123] Tassew FA, Bergland WH, Dinamarca C, Bakke R. Influences of Temperature and Substrate Particle Content on Granular Sludge Bed Anaerobic Digestion. Appl Sci 2020, Vol 10, Page 136 2019;10:136. https://doi.org/10.3390/APP10010136.

[124] Postawa K. Novel Solutions in Modeling of Anaerobic Digestion Process - Two-Phase AD Models Development and Comparison. Int J Chem React Eng 2018;16:1–16. https://doi.org/10.1515/ijcre-2017-0139.

[125] Postawa K, Szczygieł J, Kułażyński M. Heuristic methods in optimization of selected parameters of Two-Phase Anaerobic Digestion (TPAD) model. Fuel 2020;281. https://doi.org/10.1016/j.fuel.2020.118257.

[126] Rosen C, Vrecko D, Gernaey K V., Pons MN, Jeppsson U. Implementing ADM1 for plant-wide benchmark simulations in Matlab/Simulink. Water Sci Technol 2006;54:11–9. https://doi.org/10.2166/wst.2006.521.

[127] Arzate JA, Kirstein M, Ertem FC, Kielhorn E, Ramirez Malule H, Neubauer P, et al. Anaerobic Digestion Model (AM2) for the Description of Biogas Processes at Dynamic Feedstock Loading Rates. Chemie-Ingenieur-Technik 2017;89:686–95. https://doi.org/10.1002/cite.201600176.

[128] Bernard O, Hadj-Sadok Z, Dochain D, Genovesi A, Steyer JP. Dynamical model development and parameter identification for an anaerobic wastewater treatment process. Biotechnol Bioeng 2001;75:424–38. https://doi.org/10.1002/bit.10036.

[129] Sbarciog M, Giovannini G, Chamy R, Wouwer A Vande. Control and estimation of anaerobic digestion processes using hydrogen and volatile fatty acids measurements. Water Sci Technol 2018;78:2027–35. https://doi.org/10.2166/wst.2018.465.

[130] Giovannini G, Sbarciog M, Steyer JP, Chamy R, Vande Wouwer A. On the derivation of a simple dynamic model of anaerobic digestion including the evolution of hydrogen. Water Res 2018;134:209–25. https://doi.org/10.1016/j.watres.2018.01.036.

[131] Andrews JF, Graef SP. Dynamic Modeling and Simulation of the Anaerobic Digestion Process. Adv Chem 1971;105:126–62. https://doi.org/10.1021/ba-1971-0105.ch008.

[132] Wagner D, Schlüter W. Optimization of Operational Parameters in Biogas Plants using the Anaerobic Digestion Model Number 1 (ADM1) n.d. https://doi.org/10.11128/sne.30.sn.10503.

[133] Moguel-Castañeda JG, Puebla H, Méndez-Acosta HO, Hernandez-Martinez E. Modeling pH and temperature effects on the anaerobic treatment of tequila vinasses. J Chem Technol Biotechnol 2020;95:1953–61. https://doi.org/10.1002/JCTB.6361.

[134] Dalby FR, Hafner SD, Petersen SO, Vanderzaag A, Habtewold J, Dunfield K, et al. A

mechanistic model of methane emission from animal slurry with a focus on microbial groups. PLoS One 2021;16:e0252881. https://doi.org/10.1371/JOURNAL.PONE.0252881.

[135] Postawa K, Szczygieł J, Kułażyński M. Innovations in anaerobic digestion: a model-based study. Biotechnol Biofuels 2021 141 2021;14:1–11. https://doi.org/10.1186/S13068-020-01864-Z.

[136] Calise F, Cappiello FL, d'Accadia MD, Infante A, Vicidomini M. Modeling of the Anaerobic Digestion of Organic Wastes: Integration of Heat Transfer and Biochemical Aspects. Energies 2020, Vol 13, Page 2702 2020;13:2702. https://doi.org/10.3390/EN13112702.

[137] Alatiqi IM, Dadkhah AA, Jabr NM. Dynamics and Multivariable Control Analysis for Anaerobic Digestion. Chem Eng J 1990;43:B81–91. https://doi.org/10.1016/0300-9467(90)80015-5.

[138] Cazier EA, Trably E, Steyer JP, Escudie R. Biomass hydrolysis inhibition at high hydrogen partial pressure in solid-state anaerobic digestion. Bioresour Technol 2015;190:106–13. https://doi.org/10.1016/j.biortech.2015.04.055.

[139] Cazier EA, Trably E, Steyer JP, Escudie R. Reversibility of hydrolysis inhibition at high hydrogen partial pressure in dry anaerobic digestion processes fed with wheat straw and inoculated with anaerobic granular sludge. Waste Manag 2019;85:498–505. https://doi.org/10.1016/j.wasman.2019.01.019.

[140] Mairet F, Bernard O, Ras M, Lardon L, Steyer JP. Modeling anaerobic digestion of microalgae using ADM1. Bioresour Technol 2011;102:6823–9. https://doi.org/10.1016/j.biortech.2011.04.015.

[141] Oh ST, Martin AD. Thermodynamic equilibrium model in anaerobic digestion process. Biochem Eng J 2007;34:256–66. https://doi.org/10.1016/j.bej.2006.12.011.

[142] Scott S, Turra F. Six reasons to dry biogas to a low dewpoint before combustion in a CHP engine. 2013.

[143] Taifouris MR, Martín M. Multiscale scheme for the optimal use of residues for the production of biogas. Comput. Aided Chem. Eng., vol. 44, Elsevier B.V.; 2018, p. 2173–8. https://doi.org/10.1016/B978-0-444-64241-7.50357-8.

[144] Merchuk JC. Further considerations on the enhancement factor for oxygen absorption into fermentation broth. Biotechnol Bioeng 1977;19:1885–9. https://doi.org/10.1002/bit.260191211.

[145] Hepworth NJ. Characterisation of gas-liquid dispersions for beer analogues by. Imperial College London, 2003.

[146] Nedeltchev S, Schumpe A. New Approaches for Theoretical Estimation of Mass Transfer Parameters in Both Gas-Liquid and Slurry Bubble Columns. Mass Transf. Multiph. Syst. its Appl., InTech; 2011. https://doi.org/10.5772/14721.

[147] Takahashi K, McManamey WJ, Nienow AW. Bubble size distributions in impeller region in a gas-sparged vessel agitated by a rushton turbine. J Chem Eng Japan 1992;25:427–32. https://doi.org/10.1252/jcej.25.427.

[148] Hikita H, Konishi Y. Desorption of carbon dioxide from supersaturated water in an agitated vessel. AIChE J 1984;30:945–51. https://doi.org/10.1002/aic.690300609.

[149] Lekhal A, Chaudhari R V., Wilhelm AM, Delmas H. Gas-liquid mass transfer in gas-liquid-liquid dispersions. Chem. Eng. Sci., vol. 52, Elsevier Science Ltd; 1997, p. 4069–77. https://doi.org/10.1016/S0009-2509(97)00249-2.

[150] Alzate-Ibañez AM, Ocampo-Martinez C, Alzate CAC, Montoya VMT. Risk index to monitor an anaerobic digester using a dynamic model based on dilution rate, temperature, and pH.

Nonlinear Eng 2020;9:35–50. https://doi.org/10.1515/NLENG-2018-0055.

[151] Lovato G, Kovalovszki A, Alvarado-Morales M, Arjuna Jéglot AT, Rodrigues JAD, Angelidaki I. Modelling bioaugmentation: Engineering intervention in anaerobic digestion. Renew Energy 2021;175:1080–7. https://doi.org/10.1016/J.RENENE.2021.04.096.

[152] Fairlamb M, Jones R, Takács I, Bye C. FORMULATION OF A GENERAL MODEL FOR SIMULATION OF pH IN WASTEWATER TREATMENT PROCESSES n.d.

[153] Campos E, Flotats X. Dynamic simulation of pH in anaerobic processes. Appl Biochem Biotechnol 2003 1091 2003;109:63–76. https://doi.org/10.1385/ABAB:109:1-3:63.

[154] Hofmann AF, Meysman FJR, Soetaert K, Middelburg JJ. A step-by-step procedure for pH model construction in aquatic systems. Biogeosciences 2008;5:227–51. https://doi.org/10.5194/BG-5-227-2008.

[155] Capri MG, Marais G v. R. pH adjustment in anaerobic digestion. Water Res 1975;9:307–13. https://doi.org/10.1016/0043-1354(75)90052-4.

[156] Boutoute A, Di Miceli Raimondi N, Guilet R, Cabassud M, Amodeo C, Benbelkacem H, et al. Development of a Sensitivity Analysis method to highlight key parameters of a dry Anaerobic Digestion reactor model. Biochem Eng J 2021;173:108085. https://doi.org/10.1016/J.BEJ.2021.108085.

[157] Hemrajani RR, Tatterson GB. Mechanically Stirred Vessels. Handb. Ind. Mix., Hoboken, NJ, USA: John Wiley & Sons, Inc.; 2004, p. 345–90. https://doi.org/10.1002/0471451452.ch6.

[158] Vavilin VA, Angelidaki I. Anaerobic degradation of solid material: Importance of initiation centers for methanogenesis, mixing intensity, and 2D distributed model. Biotechnol Bioeng 2005;89:113–22. https://doi.org/10.1002/bit.20323.

[159] Alvarez-Cohen L, McCarty PL. Product toxicity and cometabolic competitive inhibition modeling of chloroform and trichloroethylene transformation by methanotrophic resting cells. Appl Environ Microbiol 1991;57.

[160] Feisther VA, Ulson De Souza AA, Trigueros DEG, De Mello JMM, De Oliveira D, Guelli Ulson De Souza SMA. Biodegradation kinetics of benzene, toluene and xylene compounds: Microbial growth and evaluation of models. Bioprocess Biosyst Eng 2015;38:1233–41. https://doi.org/10.1007/s00449-015-1364-0.

[161] Monod J. THE GROWTH OF BACTERIAL CULTURES. Https://DoiOrg/101146/AnnurevMi03100149002103 2003;3:371–94. https://doi.org/10.1146/ANNUREV.MI.03.100149.002103.

[162] Cheau Chin Y, Yi Jing C, Soh Kheang L, Christina Vimala S, Aik Chin S, Mei Fong C, et al. Comparison of different industrial scale palm oil mill effluent anaerobic systems in degradation of organic contaminants and kinetic performance. J Clean Prod 2020;262:121361. https://doi.org/10.1016/J.JCLEPRO.2020.121361.

[163] Moser H. The dynamics of bacterial populations maintained in the chemostat. Dyn Bact Popul Maint Chemostat 1958.

[164] Gavala HN, Angelidaki I, Ahring BK. Kinetics and Modeling of Anaerobic Digestion Process. Adv Biochem Eng Biotechnol 2003;81:57–93. https://doi.org/10.1007/3-540-45839-5_3.

[165] Contois DE. Kinetics of Bacterial Growth: Relationship between Population Density and Specific Growth Rate of Continuous Cultures. Microbiology 1959;21:40–50. https://doi.org/10.1099/00221287-21-1-40.

[166] Hashimoto AG, Chen YR, Varel VH, Prior RL. Anaerobic fermentation of animal manure. Anaerob Ferment Anim Manure 1979.

[167] Bergter F. Wachstum von Mikroorganismen — Experimente und Modelle (2. überarbeitete Auflage). 161 S., 90 Abb., 3 Tab. Jena 1983. VEB Gustav Fischer Verlag. M 61,00. Journal of Basic Microbiology, 25(1), 20–20 | 10.1002/jobm.3620250106 n.d.

[168] Mitsdoerffer R. Characteristics of two-stage thermophilic/mesophilic sludge digestion in consideration of kinetic approaches. Charakteristika der zweistufigen thermophilen/mesophilen Schlammfaulung unter Beruecksichtigung kinetischer Ansaetze 1991;no. 109.

[169] Armstrong EF. Enzymes. By J.B.S. Haldane, M.A. Monographs on Biochemistry. Edited by R.H.A. Plimmer, D.Sc., and Sir F. G. Hopkins, M.A., M.B., D.Sc., F.R.S. Pp. vii+235. London: Longmans, Green & Co., 1930. Price 14s. J Soc Chem Ind 1930;49:919–20. https://doi.org/10.1002/JCTB.5000494433.

[170] Muloiwa M, Nyende-Byakika S, Dinka M. Comparison of unstructured kinetic bacterial growth models. South African J Chem Eng 2020;33:141–50. https://doi.org/10.1016/J.SAJCE.2020.07.006.

[171] Andrews JF. A mathematical model for the continuous culture of microorganisms utilizing inhibitory substrates. Biotechnol Bioeng 1968;10:707–23. https://doi.org/10.1002/BIT.260100602.

[172] Tırınk S, Nuhoğlu A, Kul S. Investigation of the Biological Treatability of Pistachio Processing Industry Wastewaters in a Batch-operated Aerobic Bioreactor 2021. https://doi.org/10.21203/RS.3.RS-448821/V1.

[173] Alcaraz-Gonzalez V, Gonzalez-Alvarez V. On the Importance of Modeling, Optimization, and Control of Anaerobic Degradation Processes for the Treatment of Agricultural Wastewaters: Toward a Biorefinery Challenge. Towar Water Secur Soc 2021:51–61. https://doi.org/10.1007/978-3-030-50653-7_4.

[174] GRANT DJW. Kinetic Aspects of the Growth of Klebsiella aerogenes with Some Benzenoid Carbon Sources. Microbiology 1967;46:213–24. https://doi.org/10.1099/00221287-46-2-213.

[175] van den Heuvel JC, Beeftink HH, Verschuren PG. Inhibition of the acidogenic dissimilation of glucose in anaerobic continuous cultures by free butyric acid. Appl Microbiol Biotechnol 1988 291 1988;29:89–94. https://doi.org/10.1007/BF00258357.

[176] Holzberg I, Finn RK, Steinkraus KH. A kinetic study of the alcoholic fermentation of grape juice. Biotechnol Bioeng 1967;9:413–27. https://doi.org/10.1002/BIT.260090312.

[177] Miller K V., Block DE. A review of wine fermentation process modeling. J Food Eng 2020;273:109783. https://doi.org/10.1016/J.JFOODENG.2019.109783.

[178] Aiba S, Shoda M, Nagatani M. Kinetics of product inhibition in alcohol fermentation. Biotechnol Bioeng 1968;10:845–64. https://doi.org/10.1002/BIT.260100610.

[179] Parsons R V., McDuffie NG, Din GA. pH INHIBITION OF YEAST ETHANOL FERMENTATION IN CONTINUOUS CULTURE. Biomass Convers Technol 1987:73–6. https://doi.org/10.1016/B978-0-08-033174-4.50014-7.

[180] Zwietering MH, De Koos JT, Hasenack BE, De JC, Van ' K, Riet T. Modeling of Bacterial Growth as a Function of Temperature Downloaded from. Appl Environ Microbiol 1991;57:1094–101.

[181] Jun YS, Yu SH, Ryu KG, Lee TJ. Kinetic study of pH effects on biological hydrogen production by a mixed culture. J Microbiol Biotechnol 2008;18:1130–5.

[182] Borja R, Rincón B. Biogas Production ☆. Ref. Modul. Life Sci., Elsevier; 2017. https://doi.org/10.1016/B978-0-12-809633-8.09105-6.

[183] Hashimoto AG, Varel VH, Chen YR. Ultimate methane yield from beef cattle manure: Effect

of temperature, ration constituents, antibiotics and manure age. Agric Wastes 1981;3:241–56. https://doi.org/10.1016/0141-4607(81)90011-1.

[184] Unrean P. Bioprocess modelling for the design and optimization of lignocellulosic biomass fermentation. Bioresour Bioprocess 2016;3:1. https://doi.org/10.1186/s40643-015-0079-z.

[185] Birkett J, Lester J. Microbiology and Chemistry for Environmental Scientists and Engineers. CRC Press; 2018. https://doi.org/10.4324/9780203477397.

[186] Roati C, Fiore S, Ruffino B, Marchese F, Novarino D, Zanetti MC. Preliminary evaluation of the potential biogas production of food-processing industrial wastes. Am J Environ Sci 2012;8:291–6. https://doi.org/10.3844/ajessp.2012.291.296.

[187] Pavlostathis SG, Giraldo-Gomez E. Kinetics of anaerobic treatment. Water Sci Technol 1991;24:35–59. https://doi.org/10.2166/wst.1991.0217.

[188] Sanders WTM. Anaerobic hydrolysis during digestion of complex substrates. n.d.

[189] Polizzi C, Alatriste-Mondragón F, Munz G. Modeling the disintegration process in anaerobic digestion of tannery Sludge And Fleshing. Front Environ Sci 2017;5. https://doi.org/10.3389/fenvs.2017.00037.

[190] López I, Benzo M, Passeggi M, Borzacconi L. A simple kinetic model applied to anaerobic digestion of cow manure. Environ Technol (United Kingdom) 2020:1–12. https://doi.org/10.1080/09593330.2020.1732473.

[191] Luo K, Yang Q, Li X ming, Yang G jing, Liu Y, Wang D bo, et al. Hydrolysis kinetics in anaerobic digestion of waste activated sludge enhanced by α-amylase. Biochem Eng J 2012;62:17–21. https://doi.org/10.1016/j.bej.2011.12.009.

[192] Sanders WTM, Geerink M, Zeeman G, Lettinga G. Anaerobic hydrolysis kinetics of particulate substrates. Water Sci Technol 2000;41:17–24. https://doi.org/10.2166/wst.2000.0051.

[193] Vavilin VA, Fernandez B, Palatsi J, Flotats X. Hydrolysis kinetics in anaerobic degradation of particulate organic material: An overview. Waste Manag 2008;28:939–51. https://doi.org/10.1016/j.wasman.2007.03.028.

[194] Vavilin VA, Rytov S V., Lokshina LY. A description of hydrolysis kinetics in anaerobic degradation of particulate organic matter. Bioresour Technol 1996;56:229–37. https://doi.org/10.1016/0960-8524(96)00034-X.

[195] Ramirez I, Mottet A, Carrère H, Déléris S, Vedrenne F, Steyer JP. Modified ADM1 disintegration/hydrolysis structures for modeling batch thermophilic anaerobic digestion of thermally pretreated waste activated sludge. Water Res 2009;43:3479–92. https://doi.org/10.1016/j.watres.2009.05.023.

[196] Veluchamy C, Kalamdhad AS. A mass diffusion model on the effect of moisture content for solid-state anaerobic digestion. J Clean Prod 2017;162:371–9. https://doi.org/10.1016/j.jclepro.2017.06.099.

[197] Momoh YOL, Saroj DP. Development and testing of surface-based and water-based-diffusion kinetic models for studying hydrolysis and biogas production from cow manure. Renew Energy 2016;86:1113–22. https://doi.org/10.1016/j.renene.2015.09.036.

[198] Vavilin VA, Rytov S V., Lokshina LY. Two-Phase Model of Hydrolysis Kinetics and Its Applications to Anaerobic Degradation of Particulate Organic Matter. Biotechnol. Fuels Chem., Humana Press; 1997, p. 45–57. https://doi.org/10.1007/978-1-4612-2312-2_5.