Mathematical modelling of the batch anaerobic digestion process

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Abstract

The ability of anaerobic digestion to create value from waste that would not otherwise have been used, gives it a major role in the reduction of greenhouse (GHG) emissions and in the transition to a circular economy. For a better understanding of the digestion process and in order to reduce the amount of the intrinsically time-consuming laboratory tests, modelling is necessary. Current models differ in their degree of complexity. More complex models like ADM1 allow the simulation of biochemical reactions of the process. However, these models are quite difficult to calibrate as they require a high number of experimental measurements.

In that sense, an empirical model was developed to describe the kinetics of biogas production. The model was tested using experimental data generated from three batch anaerobic codigestion tests. The experimental data was accurately reproduced and the model showed a better performance than the current three-phase empirical models. In addition to the potential to reduce the amount and duration of laboratory tests, the model can also be applied as an auxiliary tool for anomaly control and mitigation of errors.

Keywords: Biogas • Anaerobic digestion • Batch • Modelling

1. Introduction

The reduction of greenhouse gas (GHG) emissions and the fight against climate change constitute one of the greatest challenges of modern world. In this context, anaerobic digestion (AD) presents itself as a technology of enormous preponderance, contributing to the achievement of the goals defined in the Paris Agreement, 2015 [1].

Anaerobic digestion can be considered a heterogeneous ecosystem where several groups of microoganisms participate interactively in the conversion of complex organic matter into biogas. According to Fagerstrom et al. [2], the biogas produced consists of a mixture of 50-70% methane (CH₄) and 30-50% carbon dioxide (CO₂). Additionally, residual amounts of gases such as: water vapor (H₂), nitrogen (N₂), hydrogen (H₂), oxygen (O2), carbon monoxide (CO), hydrogen sulphide (H₂S) and ammonia (NH₃), can be found in the final composition of biogas, depending on the substrate used and the DA process [3]. From a biochemical point of view, the DA can be described in 4 phases [4-7]: hydrolysis, acidogenesis, acetogenesis and methanogenesis (see figure 1).

With the growing interest and investment in the

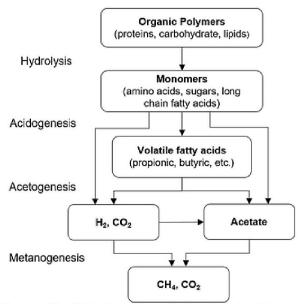


Figure 1: Simplified scheme from a biochemical point of view of the reactions that occur during the anaerobic degradation of the organic fraction of the substrate. Adapted from Shin and Song [5].

biogas production industry, it is essential to use modelling for a better understanding of the anaerobic digestion process. The determination of the kinetic constants of the system, involving different substrates, is crucial in the design of reactors and the optimization of its performance [8]. Besides, laboratory tests for AD are quite slow and expensive. Therefore, the construction of fitly calibrated mathematical models can provide an alternative in this sense, reducing the number of tests to be executed and allowing a better perception of the system's behaviour [9]. The existing analytical models of AD are divided into two groups: mechanistic or empirical. Mechanistic models such as ADM1 developed by the International Water Association [10], allow the simulation of bacteria growth and the biochemical reactions of the process. However, these models are complex and quite difficult to calibrate as they require a high number of input parameters and experimental measurements that, in most cases, are not performed in DA facilities [11]. Taking this into account, empirical models (less sophisticated) have been the object of study by several researchers [4, 11-14]. Typically, the determination of the parameters of these models requires only experimental information regarding biogas production profiles. Thus, with fewer experimental measurements compared to mechanistic models, it is possible to define the maximum potential of biogas production and the kinetics of degradation of a certain type of substrate [5, 15, 16]. However, the values obtained for the kinetic constants are rarely analyzed from a physical perspective of the process, thus lacking validation [17].

1.1. Empirical kinetic models of batch AD

Among the various empirical models available in the literature, the following stand out: the Monod model [4, 11–14] and the first order kinetic model [10, 18, 19] e o modelo cinético de 1ª ordem [15, 20–23].

The Monod model takes into account the saturation effects of the bacterial growth rate due to the limited presence of nutrients in the substrate. This model is suitable for homogeneous bacterial populations [11] and is based on mechanistic models such as MantisAD [19]. However, the Monod model is not suitable for more complex substrates with heterogeneous bacterial populations, such as municipal waste [24]. In reactors fed with particulate substrates, i.e., when hydrolysis is the limiting step of the process, the kinetics of substrate degradation follows a 1st order model [16], according to the following equation:

$$\frac{dS}{dt} = -k \cdot S_t \tag{1}$$

Where k is the degradation rate of the substrate [d⁻¹], and S_t the substrate concentration at instant t [g/L]. Thus, from a process engineering perspective, the complex system of biochemical and biological interactions that constitutes the AD can be simplified in a mechanism of one or more phases, described by 1st order kinetic reactions (see figure 2).

Single-phase models are the most common and describe the degradation of the organic fraction of the substrate in a single 1st order reaction. These models have been applied by several authors such as: Koch et al. [25], Mata-Alvarez et al. [26], Angelidaki et al. [15] or Rao and Singh [27], and allow to obtain a reasonable estimate of the temporal progression of biogas produced.

Generally, multiphase models allow to describe the temporal conversion of the substrate into bio-

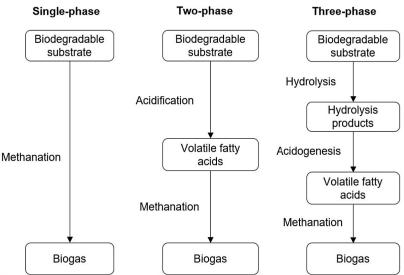


Figure 2: Reaction steps of AD from a process engineering perspective. Single-phase (left), two-phase (center) and three-phase (right) systems.

gas with more detail, providing additional information on the behavior of intermediate products formed during the AD. Shin and Song [5] describe the AD process in 2 consecutive phases of 1st order reactions: acidification and methanation. During the acidification of the biodegradable fraction of the substrate VFA are produced, which in turn are converted into biogas in the final stage of methanation.

In the scope of waste treatment from the bakery industry, Deveci and Çiftçi [28] developed a model where the AD is considered a 3 phase system, according to the diagram to the right of figure 2. This three-phase system was also applied by authors such as: Safari et al. [29], in the treatment of leachate from municipal waste; Adl et al. [8], in the production of biogas from vegetable waste and pig manure; and Zacharof and Butler [30], in the production of biogas from leachate deposited in landfills. The latter presents a modification in relation to the Deveci model, combining the 1st order kinetics of the reactions with the following growth and decay function of bacteria: $R(t) = Ate^{-kt}$, where A is a term of amplitude $[g/(L \cdot d^2)]$ and k the growth/decay rate of microorganisms [d-1].

Although they provide a reasonable estimate of the temporal progression of biogas production, both the single-phase and multiphase models mentioned above generally estimate a maximum biogas potential value lower than the last value measured in experimental tests.

Assuming that organic matter typically presents different conversion rates, Rao et al. [31] and Luna-del Risco et al. [32] developed 1st order monophase kinetic models, where the substrate is divided into two groups of components: rapidly biodegradable and slowly biodegradable. Brulé et al. [16] combined this approach with the biphasic model proposed by Shin and Song [5].

The introduction of the notion that the organic fraction of the substrate has different speeds of degradation appears to produce more realistic estimates, both in terms of the kinetics of substrate degradation and in terms of the potential of biogas produced.

2. Model development

After a revision of the empirical models proposed by different researchers to characterize the AD process, a more complete kinetic model was developed with the objective of describing the temporal degradation of the substrate along the different phases in a more precise way and to obtain more realistic estimates for the maximum potential of biogas production. The proposed model is schematically represented in figure 3, where the following assumptions were adopted:

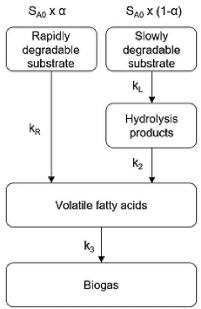


Figure 3: Schematic representation of the kinetic model of anaerobic digestion developed.

1. Organic matter has different conversion speeds and therefore the substrate can be divided into two major groups of components: rapidly biodegradable (C_R) and slowly biodegradable (C_L).

Considering the approach of Rao et al. [27] and Brulé et al. [16], this separation of the substrate into two groups can be expressed mathematically by the following equation:

$$S_A = C_R + C_L = \alpha \cdot S_{A0} + (1 - \alpha) \cdot S_{A0}$$
 (2)

Where S_A is the total concentration of biodegradable substrate, S_{A0} the initial concentration of biodegradable substrate and α the fraction of the rapidly biodegradable substrate;

- 2. The process associated with the degradation of the slowly biodegradable fraction is simplified in a system of 3 phases: hydrolysis, acidogenesis and methanogenesis, according to Deveci and Çiftçi [28]. Whereas the process associated with the rapidly biodegradable fraction is simplified in a system of only 2 phases, since this fraction is associated with the simplest monomeric compounds. S_A , S_B , S_C and S_D thus correspond to the concentrations of biodegradable substrate, products of hydrolysis, volatile fatty acids (VFA) and biogas, respectively;
- 3. Considering that both H₂ and CO₂ are rapidly consumed by methanogenic bacteria, their

role as intermediate products was considered negligible;

- 4. The reactions are considered irreversible and follow first order kinetics, which implies that the saturation effects are disregarded. k_R , k_L , k_2 and k_3 are first order kinetic constants and correspond to the degradation of the rapidly degradable substrate, the degradation of the hydrolysis products associated with the slowly degradable fraction in VFA, and the degradation of total VFA in biogas, respectively;
- 5. Due to the complexity and variability of substrate concentrations, mass balances are based on the chemical oxygen demand unit (COD) [5, 28].

Considering the assumptions adopted, the degradation kinetics along the different phases of the process is expressed by the following set of differential equations:

$$\frac{dS_A}{dt} = -\left(\alpha k_R S_A + (1 - \alpha) k_L S_A\right) \tag{3a}$$

$$\frac{dS_B}{dt} = (1 - \alpha) \left(k_L S_A - k_2 S_B \right) \tag{3b}$$

$$\frac{dS_C}{dt} = k_2 S_B (1 - \alpha) + \alpha k_R S_A - k_3 S_C \qquad (3c)$$

In order to obtain the behavior of the S_A , S_B , S_C and S_D concentrations as a function of time, the differential equations previously presented were integrated. The degradation of the organic fraction of substrate over time is thus expressed by:

$$S_A = S_{A0} \left(\alpha e^{-k_R t} + (1 - \alpha) e^{-k_L t} \right) \tag{4}$$

The intermediate function associated with the rate of accumulation of hydrolysis products from the rapidly degradable fraction of the substrate is described by:

$$S_B = S_{A0} \left[(1 - \alpha) k_L \frac{e^{-k_L t} - e^{-k_2 t}}{k_2 - k_L} \right]$$
 (5)

Then, assuming that the initial concentration of volatile fatty acids is zero, $S_C\left(t=0\right)=0$, the VFA accumulation profile as a function of time is described by:

$$S_C = S_{A0} \left[\alpha k_R \frac{e^{-k_R t} - e^{-k_3 t}}{k_3 - k_R} + (1 - \alpha) k_L k_2 \right]$$

$$\left(\frac{(k_3 - k_2) e^{-k_1 t} - (k_3 - k_1) e^{-k_2 t}}{(k_2 - k_1) (k_3 - k_1) (k_3 - k_2)} + \frac{(k_2 - k_1) e^{-k_3 t}}{(k_2 - k_1) (k_3 - k_1) (k_3 - k_2)} \right]$$

$$(6$$

The resolution of the SC function is of great interest because it allows to describe the behavior of the VFA along the anaerobic digestion. As mentioned in section 2.1, these compounds can inhibit the production of biogas and should therefore be kept at low levels to ensure better process performance. Finally, the biogas concentration results from the mass balance of the components involved in anaerobic digestion:

$$S_D = S_{A0} - S_A + S_B + S_C \tag{7}$$

Assuming that the whole substrate is converted to biogas, the maximum potential for biogas production is equal to the initial substrate concentration for an infinite retention time: $S_{A0} = S_{max}$. Thus, the function of the cumulative biogas production is expressed by:

$$S_{D} = S_{max} \left\{ \alpha \left[1 - e^{-k_{R}t} - k_{R} \frac{e^{-k_{R}t} - e^{-k_{3}t}}{k_{3} - k_{R}} \right] + (1 - \alpha) \left[1 - e^{-k_{L}t} - k_{L} \frac{e^{-k_{L}t} - e^{-k_{2}t}}{k_{2} - k_{L}} - k_{L} k_{2} \left(\frac{(k_{3} - k_{2}) e^{-k_{1}t} - (k_{3} - k_{1}) e^{-k_{2}t}}{(k_{2} - k_{1}) (k_{3} - k_{1}) (k_{3} - k_{2})} + \frac{(k_{2} - k_{1}) e^{-k_{3}t}}{(k_{2} - k_{1}) (k_{3} - k_{1}) (k_{3} - k_{2})} \right] \right\}$$
(8)

The final S_D function, which describes the cumulative production of biogas over time and its maximum potential, is thus composed of 6 parameters.

2.1. Parameter determination

In order to ensure realistic simulations in comparison with the respective experimental results, the 6 parameters of the cumulative biogas production function (S_D) should be adjusted according to the substrate used in the batch anaerobic digestion test. The unknown parameters can be determined using a numerical optimization procedure [33]. However, it is important to point out that the choice of algorithm and objective function influences the value of the estimated parameters and the accuracy of the model.

The unknown parameters were determined using the Levenberg-Marquardt algorithm [34, 35] executed in Matlab® software version 9.5.0 (R2018b) through the non-linear optimization function [Isqcurvefit]. This algorithm was chosen taking into account its suitability when solving non-linear optimization problems. In this case it consists of a least squares problem, where the set of unknown parameters (η) are iteratively determined by minimizing the objective function , which measures the

square of the difference between the experimental values (y_{exp}) and the values predicted by the model (S_D) :

$$\psi(\eta) = \min \sum_{t=0}^{N} [y_{exp}(t) - S_D(t, \eta)]^2$$
 (9)

In which N is the set of experimental measurements performed. The optimization process ends when the variation of the waste is less than the specified tolerance of 1×10^{-6} .

3. Experimental tests

In order to validate the model and to evaluate the impact on biogas production of the addition of mango to mixed sludge from conventional municipal WWTP, 3 tests were performed in a discontinuous feeding regime, with different proportions (v/v) between substrate and co-substrate: LM_{30} (70% LM, 30% LCM), LM_{10} (90% LM, 10% LCM) and LM (mixed sludge only).

The experimental tests LM₃₀, LM₁₀ and LM, were performed in series in the same order in which they were listed, in a CSTR reactor with a usable volume of 11.3 L and a storage head volume of 4.7 L. The reactor was enclosed in a thermal blanket that allowed to maintain the temperature in the mesophilic regime (37 °C \pm 1 °C). The feeding load was the same for all tests (1.13 L). The total biogas production associated with the mixture inside the reactor (biomass + feed mixture) was recorded regularly through the gas meter. As a stop criteria it was defined that the experiments were performed until the daily biogas production was less than 1% of the total production, accumulated so far, according to the general procedure proposed by Holliger et al. [36]. This way different retention times were obtained for the 3 tests: 29 days for LM₃₀, 20 days for LM₁₀ and 17 days for LM.

Table 1: Chemical characterization of the feed and digestion mixture of the LMtextsubscript30, LMtextsubscript10 and LM experimental tests.

	LM ₃₀		LM ₁₀		LM		
	In	Out		In	Out	ln	Out
рН	5,21	7,10		5,47	7,30	5,92	7,27
TS (g/L)	31,07	14,80		26,87	13,14	26,72	11,71
VS (g/L)	27,12	11,52		22,77	9,92	22,02	8,94

Subsequently, in order to check the stability and the quantity of organic matter present in the feed mixture and in the digestate, chemical analyses were carried out in terms of total solids (TS), volatile solids (VS) and pH. The concentration of TS was determined by drying the samples in the oven for a period of 24 hours at 105 °C. Then the

SV concentration was determined by placing the samples with dry residue in the furnace for a period of 8h at 550 °C [37]. The results of the chemical analyses are shown in table 1.

4. Results & discussion

4.1. Simulation of experimental tests using the developed anaerobic digestion model

The simulation results between the developed model and the experimental data of the laboratory tests performed are reproduced in the graphs of figure 4. The S_D function describes, in a very precise way, the biogas production kinetics of the 3 tests (LM₃₀: $R^2=0,9999$; LM₁₀: $R^2=0,9994$; LM: $R^2=0,9992$), then can be used as an auxiliary tool in the interpretation of data and in the detection of experimental errors.

Besides the cumulative biogas production profile, the model also allows to obtain complementary information about the temporal degradation of the mixture and the accumulation of volatile fatty acids inside the reactor (both dashed in figure 4). The measurement of these concentrations was not performed, though such a procedure would have been useful to confirm the realism of the model. However, the characteristic profiles of S_A and S_C for discontinuous regime feeding tests give a positive indication in that sense.

Analysing the mixture degradation profiles, it appears that although the LM₃₀ test complies with the stop criteria recommended by Holliger et al. [36], about 16% of the total organic matter has not been degraded, indicating that the stop criteria adopted is not the most suitable for slowly degradable mixtures. A tighter criterion is therefore recommended for these situations. As for the accumulation of VFA, the 3 tests present similar maximum values, which reflects the buffer capacity of the reactor. However, it would be expected that LM₃₀ would have a higher maximum value of accumulated VFA, followed by LM₁₀ and finally LM, since mango liquor has a high content of rapidly biodegradable organic matter, which leads to a higher initial production of VFA. The values obtained can be justified by the fact that, during the construction of the model, it was assumed that the initial VFA concentration is zero. If this concentration is known, it is recommended that when solving the dS_C/dt equation, consider that, $S_C(t=0) \neq 0$.

4.2. Error analysis

The relative error in approaching the experimental data, defined as the quotient between the residue $(y_{exp}-S_D)$ and y_{exp} , never exceeds 2.2% (maximum verified value for the LM test) and oscillates around 0, over the 3 tests, as can be seen by the graphs of the figure 4.

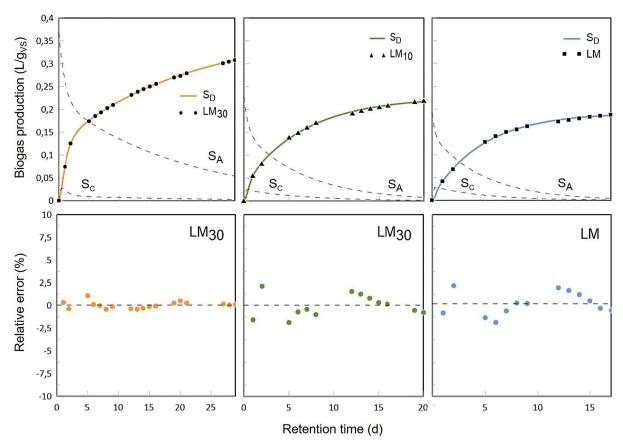


Figure 4: Simulation between the experimental data of cumulative biogas production (LM_{30} , LM_{10} and LM) and the S_D function (top). Relative error (bottom).

For the LM₁₀ and LM tests, it is possible to observe a pattern in the distribution of residues. This non-random pattern indicates that the predictive component of the model is not being able to perfectly describe part of the experimental information, with that information falling into the residuals. However, taking into account that the empirical model developed is an approximation of a complex system of biochemical processes, the results obtained are quite satisfactory.

4.3. Parameter Interpretation

The parameters of the model, obtained through the nonlinear optimization algorithm considered, are shown in table 2. From an interpretation of the values this table, the following conclusions can be drawn:

1. The S_{max} value identified by the model is higher than the last value measured experimentally, for the 3 batch tests performed. The estimate for the maximum potential of biogas produced is therefore a realistic approximation. The S_D function is therefore a valid alternative in determining the maximum potential of biogas produced, allowing to reduce the

Table 2: Optimum solution found for the parameters of the developed model.

	Parameters							
	S_{max}	k_L	k_R	k_2	k_3	α		
LM ₃₀	0,3677	0,0483	1,0135	0,8450	3,9241	0,4040		
LM_{10}	0,2267	0,1507	2,1467	1,8082	5,8215	0,3235		
LM	0,1919	0,2062	4,5113	3,8514	9,1726	0,2469		

time of experimental tests through extrapolations to infinite retention times.

- 2. The hierarchy of values registered for parameter α is coherent. Taking into account that the mango liquor has a high content of rapidly biodegradable components, namely sugars, it would be expected that the LM₃₀ test would record the highest value of α , followed by LM₁₀ and finally LM, since no co-substrate has been added to this trial.
- 3. The kinetic constant k_L registers the lowest value in every test, and therefore hydrolysis is the determining step of the process. This result is in accordance with the expected, taking into account the nature of the substrate in

question (mixed sludge).

4. The kinetic constants $(k_L, k_R, k_2 \text{ and } k_3)$ increase among the 3 tests, which indicates a faster degradation of the organic matter and therefore shorter retention times. This situation is perceptible in the graph of figure 5.

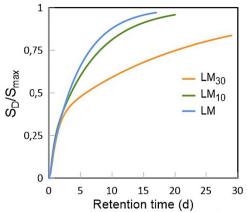


Figure 5: Biogas production kinetics. Normalised values.

The increase in the overall kinetics of biogas production verified between the 3 trials is explained on the basis that they were performed in series, which led to a progressive decay of the population of microorganisms inside the reactor and therefore a decrease in its capacity to produce biogas. On the other hand, the amount of organic matter present in the feed mixtures throughout the trials was successively smaller. With less organic matter available, the mixture inside the reactor reaches the maximum of production faster.

5. From figure 5, it can also be observed that the LM₃₀ test registers a rapid production of biogas during the first days, followed by a much slower production comparatively with the other two tests. This difference is justified by the fact that LM₃₀ was the first test to be carried out after the reactor was stopped, which was working in a continuous feeding regime, with a greater amount of organic matter available to be biodegraded. Although the identified parameters produce an estimate consistent with the experimental data, they should be reviewed for a larger number of trials. Given the variability of chemical composition of the mixture inside the reactor, it is necessary to define a reasonable range of values for the constants, in which it is possible to characterize that same mixture in a more reliable way.

4.4. Performance analysis

After being used in the interpretation of the laboratory results, the developed model was compared to

the most complete (three-phase) empirical models that have been found in the literature. In Figure 6 it is possible to schematically observe the approach of Deveci and Çiftçi [28] and of Zacharof and Butler [30].

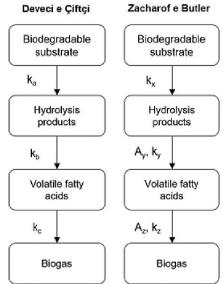


Figure 6: Schematic representation of three-phase kinetic models.

The three-phase model of Deveci and Çiftçi has the advantage of being composed of 4 parameters, in comparison with the 6 parameters of the proposed model. For this model, the S_D function that describes the cumulative production of biogas over time is expressed by:

$$S_{D} = S_{\text{max}} \left[1 - e^{-k_{a}t} - k_{a} \frac{e^{-k_{a}t} - e^{-k_{b}t}}{k_{b} - k_{a}} - k_{a}k_{b} \right]$$

$$\left(\frac{(k_{c} - k_{b}) e^{-k_{a}t} - (k_{c} - k_{a}) e^{-k_{b}t}}{(k_{b} - k_{a}) (k_{c} - k_{a}) (k_{c} - k_{b})} + \frac{(k_{b} - k_{a}) e^{-k_{c}t}}{(k_{b} - k_{a}) (k_{c} - k_{a}) (k_{c} - k_{b})} \right) \right]$$

$$\left(10 \right)$$

Where $k_a,\,k_b$ and k_c are the kinetic constants of the process.

The Zacharof and Butler model also consists of 6 parameters. However, the amplitude terms A_y and A_z , are eliminated during the integration of the differential equations, assuming that for an infinite retention time the concentrations of AGV and the hydrolysis products are approximately zero [30]. Thus, only the kinetic constants k_x , k_y and k_z remain, similar to the model of Deveci and Çiftçi. The S_D function for this model is expressed by:

$$S_D = S_{max} \left[1 - e^{-k_z t} \left(1 + k_z t \right) \right]$$
 (11)

This model offers the advantage of needing only 2 parameters to estimate the cumulative production of biogas (S_{max} and k_z). However, it is not possible to obtain any information about substrate degradation profiles and AGV accumulation from the S_D function. For a better understanding of the performance of both models, they were simulated with the experimental data of the LM₃₀ test. The results of this simulation can be observed in the graph of figure 7.

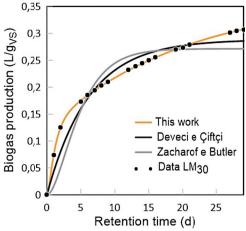


Figure 7: Comparison between the profiles of cumulative production of biogas for LM_{30} experimental test.

From the observation of the cumulative biogas production profiles it can be stated that the developed model allows the experimental information to be described more accurately. Therefore, The introduction of the concept that the organic fraction of the substrate has different degradation speeds was appropriate. On the other hand, from the estimated values for the parameters of both models, it can be noticed that both the Deveci and Çiftçi model and the Zacharof and Butler model, estimate values for the maximum potential of biogas production inferior to the last value registered experimentally. These values are shown in table 3.

Table 3: Solução ótima encontrada para os parâmetros dos modelos de Deveci e Çiftçi [28] e de Zacharof e Butler [30]. Simulação entre dados experimentais do ensaio LM_{30} e função S_D de ambos os modelos.

Model	Parameters					
Deveci e Çiftçi	S_{max}	k_a	k_b	k_c		
	0,2884	0,1623	$\gg 1$	$\gg 1$		
Zacharof e Butler	S_{max}	k_x	k_y	k_z		
	0,2714	-	-	0,3901		

Although it produces an improvement over the results obtained by the Zacharof and Butler model, the optimal solution found for the Deveci and Çiftçi model parameters suggests very high values of k_b and k_c . According to these results, the optimal so-

lution occurs when the concentrations of hydrolysis products and VFA compounds are practically zero throughout the process, which is not in agreement with reality.

Thus, it is possible to conclude that the developed model presents a better performance than the first order three-phase empirical models available in the literature, allowing a more approximate description of the experimental data recorded during the process of anaerobic digestion.

5. Conclusions

The main objective of this work was to develop an empirical model that would describe the kinetics of biogas production in batch anaerobic digestion tests, and thus allow not only a reduction in their duration, but also to act on a greater quality control. The model was tested using experimental data generated from the three batch anaerobic codigestion tests carried out. The main conclusions drawn from the work are summarized and listed below:

- 1. According to the simulation with experimental data obtained from the laboratory tests performed, the S_D function of the model developed reproduces the kinetics of biogas production accurately. The model can thus be used as an instrument to support experimental procedures.
- 2. In addition to precisely describing the experimental data, the model also provides information about the temporal degradation of the substrate (S_A) and the accumulation of VFA within the reactor (S_C) . The information related to the SC function is particularly important considering that VFA can inhibit the production of biogas, so they should be kept at low levels.
- 3. The optimal solution obtained for the parameters in the simulation with laboratory data from the tests performed is consistent with the chemical analysis performed for the feed and digested mixtures. Their interpretation proved to be of great use in understanding the behaviour of the bioreactor during the three tests. Through the normalized biogas production curves, it was possible to detect a drop in the amount of organic matter available in the biomass, caused by the fact that the tests were performed in series.
- 4. The value of S_{max} identified by the model is always higher than the last value measured experimentally, therefore producing realistic estimates for the highest potential of biogas, a

fundamental parameter in the analysis of biogas production plants performance. Taking into account the accuracy of the model in describing biogas production kinetics, the S_D function presents itself as a valid alternative to the experimental determination of the biogas potential, thus reducing the duration of experimental tests through extrapolations for infinite retention times.

 The developed model allows to describe the DA process in a more complete and precise way compared to the models within the same class, currently available.

Although the identified parameters produce an estimate consistent with the experimental data, they should be reviewed for a larger number of trials. Given the variability of the chemical composition of the mixture inside the reactor, it is necessary to define a reasonable range of values for the constants, in which it is possible to characterize the mixture more reliably.

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