

Estimation of some AM2 model parameters from a derived empirical logistic function of methane production

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Citation: Zaatri, A. (2024). Estimation of some AM2 model parameters from a derived empirical logistic function of methane production. *European Journal of Sustainable Development Research*, 8(3), em0260. <https://doi.org/10.29333/ejosdr/14637>

ARTICLE INFO

Received: 01 Feb. 2024

Accepted: 13 May 2024

ABSTRACT

Because of its capability to convert organic wastes into renewable energy and into some components useful for agriculture, the anaerobic digestion technology can reduce greenhouse gas emissions in the atmosphere and the pollution. Thus, anaerobic digestion can contribute to achieving some of sustainable development goals. Consequently, many theoretical and empirical approaches are proposed for estimating, predicting and optimizing the methane produced by anaerobic digestion. In this context, the logistic function is a mathematical model that can be used to approximate empirical data of the temporal methane production in anaerobic digestion. In a previous paper, under some appropriate approximations, we have derived from AM2 model a single analytical expression in a form of a logistic function for describing the evolution of methane production in batch bioreactors. In the present paper, by comparing the three standard parameters associated with the classical empirical logistic function with that of the derived one from AM2 model; some relationships between them have been established. These relations are exploited for estimating some coefficients and parameters of AM2 model with respect to empiric logistic function parameters and vice-versa. Moreover, this possibility enables more qualitative insight about the evolution of the methane production and the influence of AM2 parameters and coefficients as well as their interaction over its processes.

Keywords: AM2 model, anaerobic digestion, methane production, logistic model, parameters estimation

INTRODUCTION

It is well admitted nowadays that the rapid growth of the world population under the pressure of modern economic development is continually and considerably increasing the production of organic wastes. As a consequence, without appropriate management policies, organic wastes can be responsible of methane emissions, land degradation, water contamination, pollution, diseases, ecosystem destruction, etc. (Pawlita-Posmyk & Wzorek, 2018; Valenti et al., 2023). This situation heavily accentuates the climate change issues through the emission of greenhouse gases into the atmosphere. The worldwide stress of water can also be mentioned as a crucial issue and thus wastewater treatment is consequently an important topic related to waste management policies. Therefore, some recent promising research are under progress concerning wastewater treatments by using relevant techniques such as microbial metabolites in the activated sludge that govern membrane bioreactors (Sepehri & Sarrafzadeh, 2018, 2019; Sepehri et al., 2020).

For these reasons, anaerobic digestion technology is mentioned by the United Nations in the management policy of

organic wastes. It is among important technologies that can participate to reduce the impact of the climate change issues and thus contributes to achieving some sustainable development goals (Piadeh et al., 2023).

In this context, an accurate estimation, prediction and optimization of methane generation from anaerobic bioreactors is of paramount importance. In fact, since the seventies, the production of methane as a renewable energy resource generated by anaerobic bioreactors using organic wastes started attracting attention. In the same way, many research efforts have followed proposing models to estimate the methane production generated from anaerobic digesters. According to the literature review, different models have been proposed to tackle this problem based on various approaches (Emebu et al., 2022).

One very important approach is theory-based leading to mathematical expressions describing the processes acting inside the bioreactors. Some of such representative models are ADM1 and one of its derivative named AM2 (Ozgun, 2019; Yu et al., 2013). In particular, AM2 model reveals to be more practical than ADM1 and is largely used to study anaerobic digesters with different substrates in various conditions (Zaatri & Kelaiaia, 2020). But theory-based models can be

mathematically complex as they are usually composed of a set of nonlinear and coupled systems of differential equations. Thus, they cannot provide single explicit analytic expressions for estimating the evolution of the methane production, which is the final product. Instead, they are much more useful for simulating the evolution of the methane production processes. Another issue is that it is not always easy to identify and accurately estimate from experiments the many coefficients and parameters involved in these complex models (Attar & Haugen, 2019; Bernard et al., 2001; Zaatri & Kelaiaia, 2020).

To overcome this mathematical complexity and in parallel with the theory-based approach, some simplistic empirical-driven models have been proposed. These models intend to estimate the methane production by means of single explicit analytic mathematical functions that are assumed to fit their dynamic experimental profiles. For this purpose, many functions have been proposed namely Richard function, logistic function, Gompertz function, transfer function, etc. (Pererva et al., 2020; Zhang et al., 2021). Generally, these empirical-driven models involve less parameters compared to the theory-based ones. Their parameters are identified and estimated from graphical profiles of the evolution of the methane production (Opurum, 2021; Pererva et al., 2020).

Similarly, by adopting some assumptions and mathematical simplifications, some simplistic theory-based models have led to single analytic functions that met empirical-driven models. In fact, to be simplest, this type of models use different methods: such as statistical, enzymatic, kinetic, chemical, etc. (Dittmer et al., 2021; López-Aguilar et al., 2021). It was obtained by considering the steady state cases (Bernard et al., 2001), by considering the cell biomass as constant (Moharir et al., 2020), by using simple growth laws for bacteria, etc. (Bernard et al., 2001; Simeonov, 1999) or by adopting appropriate simplifications (Gouveia et al., 2022). But, because of their simplicity, this type of models cannot reflect the sensitivity of the hidden parameters influencing and governing the complex processes of real biotechnological systems.

On the other side, because of the nonlinearity of the anaerobic digestion processes and the sensitivity to their parameters and operating conditions, the simple traditional empirical-driven models may not ensure efficient performance for a generalized prediction of biogas production (Amran et al., 2024; Rutland, 2023). Therefore, some models inspired from Artificial Intelligence and modern computation techniques have recently emerged as alternatives providing better performances for biogas estimation, prediction, and even for real-time control and monitoring of bioreactors (Ling et al., 2024; Swami et al., 2023). Some of these models are machine-learning-based requiring a large amount of data. They include artificial neural networks and statistical learning models such as random forest, extreme gradient boosting, and support vector machine (Cruz et al., 2022). But, although ML models may provide better performance than classic empiric-models, they may suffer from certain limitations and challenges. These models are represented by black-boxes and their accuracy depends on the size of the data sets used to process the training and the validation phases. They also depend on the selected structure of the used ML model and from the bioreactor under consideration. These facts make them not

largely generalizable to other bioreactors operating possibly under different conditions. In addition, most applications are still lab-based and performed in batch flow rather than continuous flow bioreactors (Onu et al., 2023; Rutland, 2023). Finally, ML models are interesting but are still under progress and the comparison of their performances is not yet sufficiently mature (Amran et al., 2024; Ling et al., 2024). Finally, in the context of this research, they do not provide single analytic expressions for the evolution of the methane production and simple methods for identifying the parameters characterizing the processes of methane production.

As a conclusion, according to our critical analysis of the previous literature review, we did not find models of single analytical expressions that describe the evolution of the methane production while holding the many parameters and coefficients used in the complex models representing at least two processes such as those involved in AM2 model such as acidogenic and methanogenic processes. On the other side, the used parameters are usually limited, model dependant, and, are not always easy to estimate. Thus, they do not provide insight concerning the influence of the used parameters over the evolution of the methane production.

In effect, as a summary, firstly, the complex theory-based models such as AM1 and AM2 are mainly useful for simulation. Secondly, the empirical-driven models provide single analytical expressions but do not hold enough parameters. In addition, there parameters may not have direct meanings related to microbiological activities. Thirdly, some simplified theory-based models that have derived single analytical expressions miss most microbiological parameters and yield coefficients. Fourthly, the ML-based models do not provide single expressions as they are black-boxes.

Therefore, there is a need for new models derived from the theory-based approach that can hold some microbiological parameters and yield coefficients, but, at the same time, they may still be comparable to empiric-driven models representable with single analytic functions. Thus, according to the author's review of the literature, this vision seems to have not sufficiently investigated and that is why probably, there is almost no references corresponding precisely to this topic. However, in response to this issue, we have previously proposed two contributions. By adopting some appropriate mathematical simplifications, two single analytical expressions derived from AM2 model while holding most of its parameters have been proposed (Zaatri, 2021a, 2021b). In particular, one of these research works (Zaatri, 2021b) has proposed single analytical expressions for the evolution of the bacteria's and the methane production in batch AD. The expressions are derived from AM2 model with its main parameters and are also match the profile of logistic functions.

Actually, the main objective of the present research work aims to exploit the proposed model cited in Zaatri (2021b). Our original contribution is the establishing of relations between the experimental parameters of the logistic functions concerning the evolution of the bacteria' and the methane production with those of the theoretical ones related to AM2 model. Then, from these relations, some parameters of AM2 can be estimated in function of the experimental ones and vice-versa. This also leads to more qualitative and quantitative insight concerning the evolution of the processes leading to

the cumulated methane production as well as to the influence of AM2 parameters over these processes.

MATHEMATICAL FORMULATION OF AM2 MODEL

In this section, we briefly present the formulation of AM2 model, which belongs to the theory-based approach for estimating the cumulated methane generated by anaerobic digestion in the case of batch bioreactors. This estimation will be obtained via numerical simulations according to the adopted mathematical formulation. The obtained results provided by this formulation will serve as a reference, at least qualitatively, to compare with those of the derived data-driven model, which corresponds to a logistic function.

AM2 model considers the anaerobic digestion as constituted only of two main steps leading to the production of a biogas that contains the methane (Bernard et al., 2001). The first step involves the acidogenic bacteria to decompose the organic substrate into volatile fatty acids (VFA) and CO₂. Then, the second step involves the methanogenic bacteria to generate CO₂ and methane. S₁ represents the concentration of a soluble carbonaceous substrate while S₂ represents the concentration of VFA. X₁ and X₂ represent, respectively, the concentrations of acidogenic and methanogenic bacteria populations. We note that as we are principally interested in the estimation of the cumulated methane, and since the general set of equations of AM2 model can be decoupled, therefore the alkalinity, the pH, the flow of CO₂, or the partial pressure of the gases will not be considered (Vargas et al., 2019). On the other hand, in this study, we are concerned with the analysis of batch reactors, then the mathematical model is reduced to a set of four differential equations:

$$\frac{dX_1}{dt} = \mu_1 X_1, \quad (1)$$

$$\frac{dX_2}{dt} = \mu_2 X_2, \quad (2)$$

$$\frac{dS_1}{dt} = -k_1 \mu_1 X_1, \quad (3)$$

$$\frac{dS_2}{dt} = k_2 \mu_1 X_1 - k_3 \mu_2 X_2, \quad (4)$$

where k_1 , k_2 , k_3 , and k_4 are yield coefficients associated with the reactions. The specific reaction rates are of monod type μ_1 for acidogenesis and haldane type μ_2 for methanogenesis bacteria:

$$\mu_1 = \mu_{1max} \frac{S_1}{K_{S1} + S_1}, \quad (5)$$

$$\mu_2 = \mu_{2max} \frac{S_2}{K_{S1} + S_2 + \frac{S_2^2}{K_{i2}}}, \quad (6)$$

where μ_{1max} is the maximal growth rate and K_{S1} is the constant of half-saturation of the acidogenic biomass. μ_{2max} is the maximal growth rate, K_{S2} is the constant of saturation and K_{i2} , the constant of inhibition of the methanogenesis bacteria.

Four initial conditions $X_1(0)$, $S_1(0)$, $X_2(0)$, and $S_2(0)$ have to be, respectively, associated to the set of differential equations.

According to this model, the methane flow can be deduced from:

$$Q_{CH_4}(t) = k_4 \mu_2 X_2(t), \quad (7)$$

where k_4 is the yield coefficient for the methane production. The cumulative methane $V(t)$ generated over a period of time t is deduced, as follows:

$$V(t) = k_4 X_2(t). \quad (8)$$

This model can simulate more or less adequately the functioning of the anaerobic digesters and predict the produced methane more or less accurately depending on many factors such as the composition of the substrates, the operating conditions and the estimation of the involved parameters. For the model under interest, there are nine parameters to be identified, five of them are related to the growth processes (μ_{1max} , K_{S1} , μ_{2max} , K_{S2} , and K_{i2}) and four of them are the yield parameters (k_1 , k_2 , k_3 , and k_4). There are four initial conditions that ($X_1(0)$, $S_1(0)$, $X_2(0)$, and $S_2(0)$) could be measured or estimated depending on the bioreactor design.

The methods of parameters identification consider the bioreactor in the context of system control and use large sets of experimental data. Then, the parameters are estimated according to criteria's that should minimize functions of errors between the theoretical and the experimental values (Attar & Haugen, 2019; Bernard et al., 2001).

LOGISTIC FUNCTION AS A MODEL FOR METHANE PRODUCTION

In this section, we present the logistic function, which is used for estimating the cumulated methane generated by anaerobic digestion and which belongs to the data-based approach. The logistic function is a mathematical expression, which is used to modeling many domains of applications such as biomathematics, chemistry, physics, demography, economics, etc. In particular, it is used to study a population growth under conditions of limited resources (Di Crescenzo & Paraggio, 2019).

The logistic equation emerges as a solution of a first order differential Eq. (9), where the function $X(t)$ represent the growth population, given a growth rate, c , and a carrying capacity, a .

$$\frac{dX}{dt} = cX \left(1 - \frac{X}{a}\right). \quad (9)$$

It has also associated to an initial value that is the initial population: $X(0)=X_0$.

The logistic function is usually expressed in the following two forms, where the function is represented by $X(t)$ while t is the independent variable and (a , b , and c) or (a , β , and c) are its parameters.

The first expression of the logistic function is, as follows:

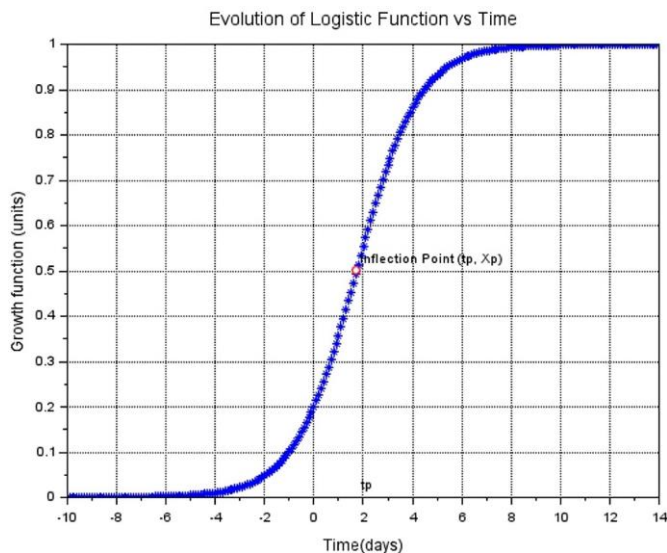


Figure 1. Logistic function (Source: Author's own elaboration)

$$X(t) = \frac{a}{1+b \times \exp(-ct)}. \quad (10)$$

The second form is also known as Ratkowsky expression is, as follows:

$$X(t) = \frac{a}{1+\exp(\beta-ct)}, \quad (11)$$

with $b=e^\beta$ and $b>0$ and $c>0$.

The shape of this function increases for $t \geq 0$ and has a horizontal asymptote when t tends to an infinite value that is the capacity= a (Figure 1). It has also an inflexion point with coordinates (t_p, x_p) . It corresponds to the time t_p , where X_p reaches the half value of the carrying capacity.

Once a graphical experimental profile of the logistic function $X(t)$ is given, its parameters (a , b , and c) can be determined based on some particular points from the experimental curve. The first coefficient to be determined is the carrying capacity a that corresponds to the asymptotic value for time to infinite time. In Figure 1, it is about unity. The second parameter b is related to the initial value of the logistic function X_0 and is determined by from the following expression:

$$b = \frac{a-X_0}{X_0}. \quad (12)$$

The growth rate parameter c is deduced from the coordinates of the inflexion point. It corresponds to the time t_p , where X_p reaches the half value of the carrying capacity. Thus, when $X_p=a/2$, the time is $t_p=(1/c)\log(b)$, and then:

$$c = \frac{1}{t_p} \log(b). \quad (13)$$

To give meanings to the parameters of the logistic function modeling cumulated methane production by microbiological activities, a specific re-parameterization is defined in the following third form (Oporum, 2021):

$$X_t = \frac{A}{(1+\exp(-\frac{4v_{max}}{A}(t-\lambda)+2))}, \quad (14)$$

where for instance $X(t)$ represents the cumulated methane produced over a time duration t , A the maximum product, v_{max} is the maximum production rate, and λ the lag phase time.

EVOLUTION OF ACIDOGENS BACTERIA AS LOGISTIC FUNCTION

Approximation of Evolution of Bacteria $X_1(t)$ by a Logistic Function

The dynamic evolution of bacteria $X_1(t)$ can be derived from combining Eq. (1) and Eq. (5), which leads to the following differential equations (Zaatri, 2021b):

$$\frac{dX_1}{dt} = \mu_{1m} \frac{S_1}{S_1+K_{S1}} X_1 = \mu_{1m} \frac{(-k_1 X_1 + \alpha) X_1}{(-k_1 X_1 + K_{S1} + \alpha) X_1}, \quad (15)$$

with $\alpha=S_{10}+k_1 X_{10}$. This equation can be solved and expressed as an algebraic equation but without explicit solution in function of time.

However, it can be expressed in the inverse form: $t=g(X_1)$ (Zaatri, 2021a). Nevertheless, by considering an approximation that is $(k_1 X_1 < \alpha + K_{S1})$, Eq. (15) simplifies such as:

$$\frac{dX_1}{dt} = \mu_{1m} \frac{(-k_1 X_1 + \alpha) X_1}{K_{S1} + \alpha} = \frac{\alpha \mu_{1m}}{\alpha + K_{S1}} \left(1 - \frac{\alpha}{k_1} X_1\right) X_1. \quad (16)$$

One can notice that Eq. (16) corresponds formally to Eq. (9), therefore, $X_1(t)$ can be expressed as a logistic function, as follows:

$$X_1(t) = \frac{\alpha}{k_1} \frac{1}{1 + \frac{S_{10}}{k_1 X_{10}} \exp\left(-\frac{\alpha \mu_{1m} t}{\alpha + K_{S1}}\right)}. \quad (17)$$

A similar expression has been obtained in Zaatri (2021a) with a little difference in the adopted approximation. Eq. (17) has the form of a logistic function as in Eq. (10). Comparing the obtained theoretical approximated Eq. (17) with assumed experimental logistic functions as defined in Eq. (10) and Eq. (11) with the parameters (a , b , and c), it gives the following relations:

$$\alpha_1 = \frac{\alpha}{k_1} = X_{10} + \frac{S_{10}}{k_1}, \quad b_1 = \frac{S_{10}}{k_1 X_{10}}, \quad c_1 = \alpha \frac{\mu_{m1}}{(\alpha + K_{S1})}. \quad (18)$$

If we consider the parameterization as defined by Eq. (11), it gives the following relations:

$$\alpha_1 = \frac{\alpha}{k_1} = X_{10} + \frac{S_{10}}{k_1}, \quad b_1 = e^{\beta_1}, \quad c_1 = \alpha \frac{\mu_{m1}}{(\alpha + K_{S1})}. \quad (19)$$

If again we consider the parameterization as defined by Eq. (14), it gives the following relations:

$$A_1 = a_1 = \frac{\alpha}{k_1} = X_{10} + \frac{S_{10}}{k_1},$$

$$\lambda_1 = \frac{\beta-2}{c_1} = \frac{\log(b_1)-2}{c_1} = \frac{(\log(b_1)-2)(\alpha+K_{S1})}{\alpha} \frac{1}{\mu_{m1}}, \quad (20)$$

$$v_{1max} = \frac{a_1 c_1}{4} = \frac{\alpha^2}{4k_1(\alpha+K_{S1})} \mu_{m1}.$$

Inversely,

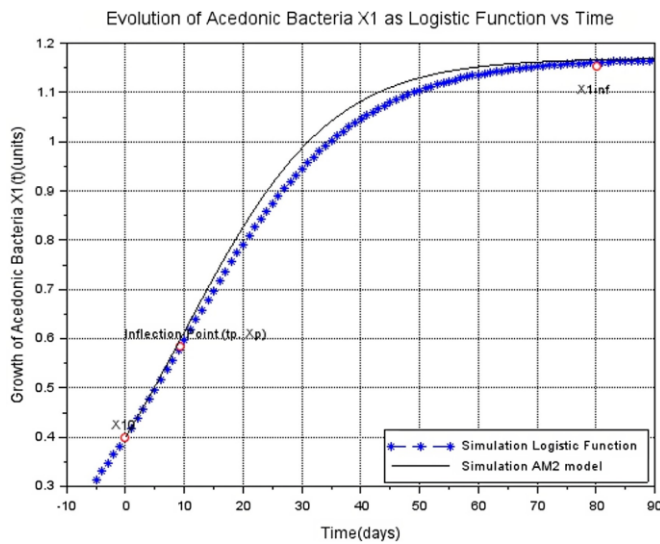


Figure 2. Analytical expression of $X_I(t)$ as a logistic function (Source: Author's own elaboration)

$$\alpha_1 = A_1, \quad b_1 = e^{\frac{4V_{1max}}{A_1} + 2}, \quad c_1 = 4 \frac{V_{1max}}{A_1}. \quad (21)$$

Figure 2 presents the simulation, by means of the software Scilab, of $X_I(t)$ according to AM2 model, which is the black curve. The curve with blue stars represents $X_I(t)$ obtained from the analytical Eq. (17), which is a logistic function.

The three remarkable points enabling to extract graphically the parameters (a_i , b_i , and c_i) from the supposed experimental curve are shown with red circles. The first point corresponds to the initial concentration at $t=0$, which is $X_{I0}=0.4$ mg/l. The second is the inflection point ($t_p=9.37$ days, $X_I=0.58$ mg/l). The third one corresponds to the steady state condition that is X_{Iinf} , which tends to maximal value $a_i=1.17$ mg/l reached after about 70 days. By calculations from the given values of AM2 model ($U_{m1}=0.4$ day $^{-1}$; $K_{S1}=72$ mg/l; $k_i=13$; $X_{I0}=0.4$ mg/l; and $S_{I0}=10$ mg/l); the numerical values of the parameters for the three type of logistic functions are ($a_i=1.17$ mg/l; $b_i=1.92$; $c_i=0.07$ day $^{-1}$). The parameter for the second form are ($a_i=1.17$ mg/l; $\beta_i=0.65$; and $c_i=0.07$ day $^{-1}$). The parameters for the third one are ($a_i=1.17$ mg/l; $\lambda_i=-19.30$; and $V_{max}=0.02$ day $^{-1}$).

Comments

The logistic function obtained in Eq. (17) by approximations can help to analyze the dynamic behavior of the acetogenic population $X_I(t)$ with respect to the corresponding AM2 parameters (U_{1m} , K_{S1} , and k_i) and the initial values (S_{I0} and X_{I0}). The comparison of the empiric logistic function in Eq. (10), Eq. (11), and Eq. (14) with our approximated analytical logistic function in Eq. (17) leads to the following remarks.

All parameters (a_i , b_i , and c_i) depend on the initial conditions (S_{I0} and X_{I0}). The asymptotic value a_i depends linearly on the initial conditions (S_{I0} and X_{I0}) and on the yield coefficient k_i . Thus, the maximal production of acidogenic bacteria $X_I(t)$ that corresponds to a_i can be increased by increasing the initial values of X_{I0} , S_{I0} , and decreasing k_i . The intersection of $X_I(t)$ with the vertical axis, which is X_{I0} is related to b_i and is influenced by the parameters (X_{I0} , S_{I0} , and k_i). Only the parameter c_i depends, beside the parameters (X_{I0} , S_{I0} , and

k_i), on the growth parameters (U_{m1} and K_{S1}). Therefore, for batch bioreactors, by selecting the substrate and bacteria, it becomes possible to control the evolution of $X_I(t)$.

However, if we consider the third form of logistic function in Eq. (14); then, only $A_i=a_i$ depends on the initial values as for the other types. But both the lag phase time λ and the maximum production rate V_{max} are influenced by the growth parameters (U_{m1} and K_{S1}). These last relations reveals that λ depends in an inverse linear way on the maximal growth rate (U_{m1}) while V_{max} depends on it linearly.

Identification of AM2 Parameters from Logistic $X_I(t)$ Profile

If one considers the parameters (a_i , b_i , and c_i) of a logistic function as estimated from experimental data; then, by inverting and manipulating Eq. (18), one can infer an estimation of some parameters of AM2 model. For instance, by assuming that the yield coefficient k_i is determined by any means, then, the initial conditions concerning the bacteria's and the substrate (X_{I0} and S_{I0}), as well as the parameter of growth rate (U_{m1}) can be identified with respect to the empirical parameters (a_i , b_i , and c_i):

$$X_{I0} = \frac{a_i}{1+b_i}, \quad S_{I0} = k_i \frac{a_i b_i}{1+b_i}, \quad U_{m1} = \frac{K_{S1} + k_i a_i c_i}{k_i a_i}, \quad (22)$$

These relations reveals that X_{I0} can be estimated from (a_i and b_i) but S_{I0} and V_1 require the determination of k_i . Moreover, S_{I0} is proportional to k_i while U_{m1} is inversely proportional to k_i . In addition, these parameters (X_{I0} , S_{I0} , and U_{m1}) can also be expressed with respect to the biological parameters (A_1 , λ_1 , and V_{1max}) using relations in Eq. (20) and Eq. (21).

Approximation of Dynamic Degradation of Substrate $S_I(t)$

The dynamic degradation of the substrate $S_I(t)$ can be derived from combining Eq. (1) and Eq. (3), which leads to the following differential equations (Zaatri, 2021b):

$$\frac{dS_I}{dt} = -k_1 \frac{dX_I}{dt}. \quad (23)$$

By integrating Eq. (23) and replacing $X_I(t)$ from Eq. (17), the substrate degradation $S_I(t)$ can also be derived in the form of a logistic function:

$$S_I(t) = -k_1 X_I(t) + \alpha = \frac{-\alpha}{(1 + \frac{S_{I0}}{k_1 X_{I0}} \exp(-\frac{\alpha U_{m1}}{\alpha + K_{S1}} t))}. \quad (24)$$

Figure 3 presents the simulation, by means of the software Scilab, of $S_I(t)$ according to AM2 model, which is the black curve. The curve with blue stars represents $S_I(t)$ obtained from the analytical expression in Eq. (17), which is related to a logistic function via $X_I(t)$.

The three remarkable points enabling to extract graphically the parameters (a_{IS} , b_{IS} , and c_{IS}) from the supposed experimental curve are shown with red circles. The first point corresponds to the initial concentration at $t=0$, which is $S_{I0}=10$.

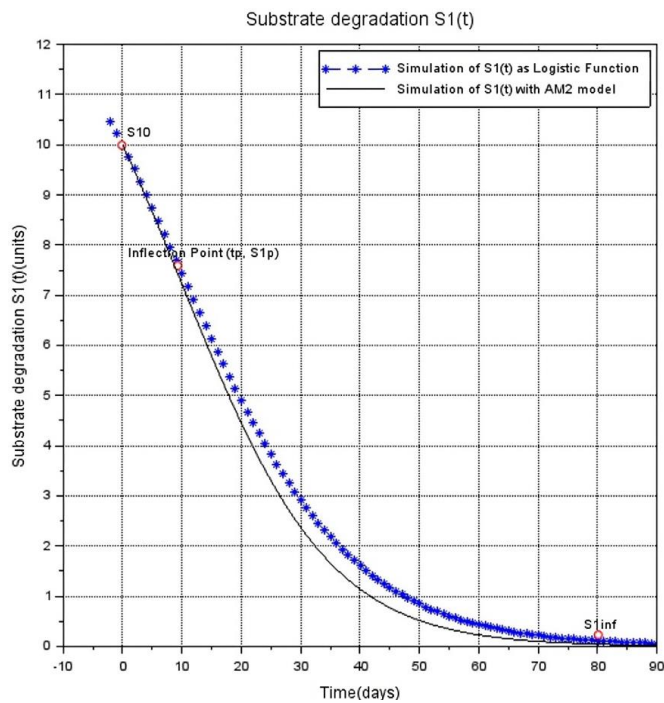


Figure 3. Analytical expression of $S_I(t)$ (Source: Author's own elaboration)

The second is the inflection point ($t_p=9.37$ and $S_I=7.6$). The third one corresponds to the steady state condition that is S_{Iinf} , which tends to the minimal value, which is about zero reached after about 70 days and which means that the substrate are almost completely consumed by the acidogenic bacteria populations.

We notice that since $S_I(t)$ is directly linked to the logistic function $X_I(t)$, then relations in Eq. (16) and Eq. (21) can be used to estimate some parameters or group of parameters of AM2 model.

If it is possible to obtain such curve from experimental measures, therefor S_{10} , which is the initial substrate can be easily measured or estimated from the beginning.

EVOLUTION OF METHANOGENS BACTERIA AS LOGICAL FUNCTION

From Eq. (2) and Eq. (4) of the differential equations of AM2 model, we can write:

$$\frac{dX_2}{dt} = \mu_2 X_2 = \mu_{2max} \frac{S_2}{S_2 + \frac{S_2^2}{K_{I2}} + K_{S2}} X_2. \quad (25)$$

On the other hand, as shown in paper (Zaatri, 2021b), by manipulating and inserting Eq. (1), Eq. (2), and Eq. (4) in Eq. (25), we can obtain a nonlinear differential equation of the first order on $X_2(t)$, which depends on $X_1(t)$ via the term $f(t)$ such as:

$$\frac{dX_2}{dt} = u_{m2} \frac{(-k_3 X_2 + f) X_2}{((-k_3 X_2 + f) + \frac{(-k_3 X_2 + f)^2}{K_{I2}} + K_{S2})} = g(X_2, X_1), \quad (26)$$

with $f(t)=k_2 X_1(t)+C$ and $C=S_{20}-k_2 X_{10}+k_3 X_{20}$.

One way to provide an analytical solution to Eq. (26) consists, as shown in Zaatri (2021b) to make some approximations. The first step requires the adoption of a simplified growth law for the methanogenic process such as Blackman's model (Blackman, 1911), which is, as follows:

$$\mu_2 = \frac{u_{m2}}{K_{S2}} S_2. \quad (27)$$

This approximation means that the growth law is relatively valid at the beginning of the growth process. By adopting this approximation; Eq. (25) and Eq. (26) can be written, as follows:

$$\frac{dX_2(t)}{dt} \cong u_{m2} \frac{S_2(t)}{K_{S2}} X_2 = \frac{u_{m2}}{K_{S2}} f(t) X_2(t). \quad (28)$$

Eq. (28) can be rewritten to match the standard form of Bernoulli's differential equation for the particular case, where the coefficient $n=2$ (Parker, 2020), that is:

$$\frac{dy(t)}{dt} + P(t)y(t) = Q(t)y^2(t). \quad (29)$$

By identification Eq. (28) to Eq. (29), one gets $P(t)$ and $Q(t)$:

$$P(t) = -\frac{u_{m2}}{K_{S2}} (C + k_2 X_1(t)), \quad Q(t) = q_0 = -\frac{u_{m2}}{K_{S2}} k_3. \quad (30)$$

The differential Eq. (29) has a general solution (Parker, 2020):

$$y(t) = \frac{e^{\int_0^t P(t) dt}}{c_0 - q_0 \int_0^t e^{\int_0^t P(t) dt} dt}. \quad (31)$$

To explicit the general solution of Eq. (31), it requires the provision of $P(t)$, which means to provide the profile of $X_1(t)$. Here again, the problem of integrating Eq. (31) is not obvious in standard analytical expressions. So, a second approximation is made that is to use the expression of a logistic function for $X_1(t)$ as given by Eq. (17). Then, a third and last simplification is necessary and consists of neglecting the terms that vanished for relatively large values of time t in the solution of Eq. (28) (Zaatri, 2021b). Within these approximations, the evolution of the methanogens bacteria can then be amenable in the form of a logistic function with respect to AM2 parameters, as follows:

$$X_2(t) \cong \frac{p_0 + p_1}{q_0} \frac{1}{(1 + E_1 \exp(p_0 + p_1)t)}, \quad (32)$$

with $p_0 = -\frac{u_{m2}}{K_{S2}} C$, $p_1 = -\frac{u_{m2}}{K_{S2}} k_2 \frac{\alpha}{k_1} = -\frac{u_{m2}}{K_{S2}} \frac{k_2}{k_1} (S_{10} + k_1 X_{10})$, $q_0 = -\frac{u_{m2}}{K_{S2}} k_3$, and $E_1 = \frac{p_0 + p_1}{q_0 X_{20} (1 + b_1) c_1} - 1$.

By means of Eq. (32), one can identify the parameters of the Logistic function from the experimental data of the methanogens bacteria growth profile for any type of the three used forms. Using Eq. (10) of the logistic function, one can establish the relations between its experimental parameters (a_2 , b_2 , and c_2) with those of AM2 model given by Eq. (32), which are:

$$a_2 = \frac{p_0 + p_1}{q_1} = \frac{1}{k_3} \left(\frac{k_2}{k_1} S_{10} + S_{20} + k_3 X_{20} \right),$$

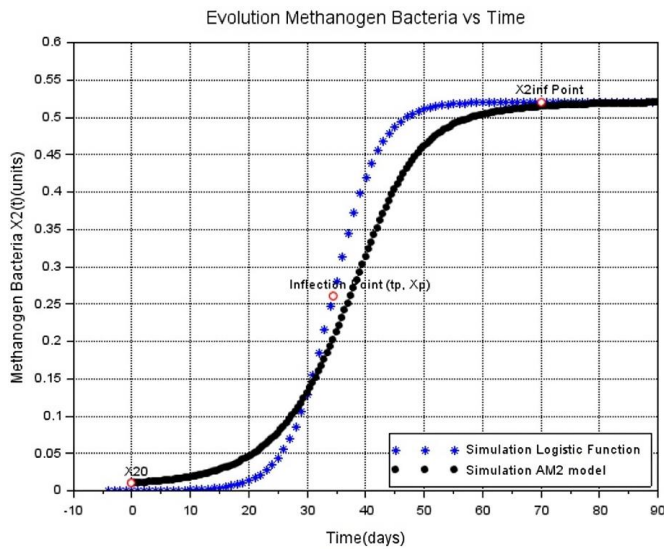


Figure 4. Analytical expression of $X_2(t)$ as a logistic function (Source: Author’s own elaboration)

$$b_2 = E_1 = \left[\frac{p_0 + p_1}{q_0} \frac{(1+b_1)^{\frac{p_1}{c_1}}}{X_{20}} - 1 \right], \tag{33}$$

$$c_2 = -(p_0 + p_1) = \left(\frac{k_2}{k_1} S_{10} + S_{20} + k_3 X_{20} \right) \frac{u_{m2}}{K_{S2}}$$

Figure 4 presents the simulation, by means of the software Scilab, of $X_2(t)$ according to AM2 model, which is the black curve. The curve with blue stars represents $X_2(t)$ obtained from the analytical Eq. (32), which corresponds to a logistic function.

Given the values of AM2 model concerning the methanogen bacteria, which are ($U_{m2}=0.4 \text{ day}^{-1}$; $K_{S2}=72 \text{ mg/l}$; $k_2=12$; $k_3=22$; $X_{20}=0.01 \text{ mg/l}$; and $S_{20}=2 \text{ mg/l}$), the parameters of the logistic function in Eq. (30) can be determined according to Eq. (33): $a_2=0.52 \text{ mg/l}$; $b_2=6302.10$; $c_2=0.25 \text{ day}^{-1}$.

Its three remarkable points enabling to extract graphically the parameters (a_2 , b_2 , and c_2) are shown with red circles. The first point corresponds to the initial concentration at $t=0$, which is $X_{20}=0.01 \text{ mg/l}$; the second to the inflection point ($t_{2p}=38.10 \text{ days}$; $X_{2p}=0.26 \text{ mg/l}$); and the third one to the steady state point is $X_{2inf}=0.52 \text{ mg/l}$ since t_{2inf} about 70 days.

Because the initial conditions are arbitrarily chosen, the parameter b_2 given in Eq. (33) does not necessarily match the initial conditions of the differential Eq. (12). However, it corresponds to an equivalent initial value X_{2eq} that depends on a complex combination of AM2 parameters, as follows:

$$b_2 = E_1 = \left[\frac{p_0 + p_1}{q_0} \frac{(1+b_1)^{\frac{p_1}{c_1}}}{X_{20}} - 1 \right], \tag{34}$$

where $X_{2eq} = X_{20} \left(1 + b_1 \right)^{\frac{p_1}{c_1}} = X_{20} \left(1 + \frac{S_{10}}{k_1 X_{10}} \right)^{\frac{p_1}{c_1}}$.

ESTIMATION OF METHANE PRODUCTION BY A LOGISTIF FUNCTION

Logistic Function Modeling for Cumulated Methane Production $V(t)$

According to AM2 model, the cumulated methane production $V(t)$ is directly proportional to the growth of methanogens bacteria $X_2(t)$ as in Eq. (8). Derived from Eq. (32), the cumulated methane production can be expressed in any of the three logistic function in Eq. (10), Eq. (11), and Eq. (14). Therefore, it follows:

$$V(t) = k_4 X_2(t) \cong k_4 \frac{p_0 + p_1}{q_0} \left(\frac{1}{1 + E_1 \exp(p_0 + p_1)t} \right). \tag{35}$$

This expression $V(t)$ corresponds to a logistic function that has been used for predicting the cumulative methane production by many authors (Di Crescenzo & Paraggio, 2019). Let’s compare $V(t)$ of Eq. (35) with the logistic function in the following form of Eq. (10):

$$V(t) = k_4 \frac{p_0 + p_1}{q_0} \left(\frac{1}{1 + E_1 \exp(p_0 + p_1)t} \right) = \frac{A_m}{(1 + B_m \exp(-\frac{C_m}{t}))}, \tag{36}$$

where $V(t)$ is the methane volume cumulated during time t and (A_m , B_m , and C_m) are the three parameters that characterize the behavior of $V(t)$. They have to be determined via a graphical representation profile obtained from a set of experimental data.

Determination of Parameters of Logistic Function $V(t)$

By comparing the expressions in both side of Eq. (36), we can establish relationships between the parameters of the two models. The empirical parameters (A_m , B_m , and C_m) expressed in terms of the approximate AM2 proposed model can be written as:

$$A_m = k_4 \frac{p_0 + p_1}{q_0} = \frac{k_4}{k_3} \left(\frac{k_2}{k_1} S_{10} + S_{20} + k_3 X_{20} \right),$$

$$B_m = E_1 = \left[\frac{p_0 + p_1}{q_0} \frac{(1+b_1)^{\frac{p_1}{c_1}}}{X_{20}} - 1 \right] = \frac{1}{k_3} \left(\frac{k_2}{k_1} S_{10} + S_{20} + k_3 X_{20} \right) \frac{1}{X_{20}} \frac{1}{(1 + b_1)^{\frac{p_1}{c_1}} - 1}, \tag{37}$$

$$C_m = p_0 + p_1 = \left(\frac{k_2}{k_1} S_{10} + S_{20} + k_3 X_{20} \right) \frac{u_{m2}}{K_{S2}}$$

Figure 5 presents the simulation, by means of the software Scilab, of $V(t)$ according to AM2 model, which is the black curve. The curve with blue stars represents $V(t)$ obtained from the analytical Eq. (35), which is a logistic function. The value of the coefficient k_4 is assumed to be equal to $75 \text{ l}^2/\text{mg}$.

The three remarkable points enabling to graphically extract the logistic function parameters (A_m , B_m , and C_m) are shown with red circles. The inflection point is ($t_{2p}=34.38 \text{ day}^{-1}$; $V_{2p}=19.52 \text{ l}$). The steady state point starts from about $t_{2inf}=65 \text{ days}$ and corresponds to the maximum accumulated methane, which is about $V_{2inf}=39 \text{ l}$. The initial point corresponding to the initial accumulation at $t=0$ does not necessarily match the

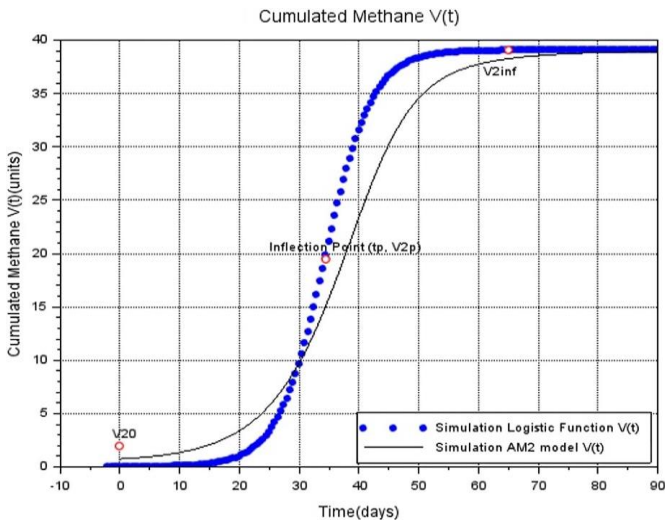


Figure 5. Profile of approximate logistic function derived from AM2 model for cumulated methane production (Source: Author's own elaboration)

initial arbitrary given value related to S_{20} that is ($V_0=k_4X_{20}=0.75$ l) but correspond to the equivalent initial condition, as shown in Eq. (32) that is ($V_{0equ}=k_4X_{20equ}=0.006$ l), which is negligible. Based on the parameter values of AM2 model, the logistic function parameters are: $A_m=39.036$ l; $B_m=2731.715$; and $C_m=0.254$ day⁻¹.

Some Comments About Logistic Function Representing Cumulated Methane

The parameter A_m represents the highest value reached by the cumulated methane production. According to relation (37), it depends on the coefficients (k_1, k_2, k_3 , and k_4) and on the initial values (S_{10}, S_{20} , and X_{20}). Therefore, to increase and optimize the methane production in batch reactors, one should select the input products and settle the initial conditions in the following way. Increase k_2 and k_4 while decreasing k_1 and k_3 . Increase S_{10}, S_{20} , and X_{20} , by selecting the nutriment and initial conditions. The parameter C_m represents the production rate, according to its expression in Eq. (37), it is related to yield coefficients and initial conditions plus the growth rate U_m and K_{S2} . The evolution of the cumulated methane production is then led by the initial conditions and the growth parameters of the methanogens bacteria.

If we consider, the modified logistic function $V_m(t)$ in the form of Eq. (14), then, Eq. (35) can be written:

$$V(t) \cong k_4 \frac{p_0+p_1}{q_0} \left(\frac{1}{1+E_1 \exp(p_0+p_1)t} \right) = \frac{A}{(1+\exp(-\frac{4V_{max}}{A})(t-\lambda)+2)} \tag{38}$$

This re-parameterization involves the maximum methane production (A), the duration of the lag phase (λ), and the maximum rate of methane production (V_{max}). By comparing the two sides of Eq. (38), the parameters of the modified logistic function (A, V_{max} , and λ) can be expressed in terms of the approximate AM2 model parameters, as follows:

$$A = k_4 \frac{p_0+p_1}{q_0} = \frac{k_4}{k_3} \left(C + \frac{k_2}{k_1} a \right) = \frac{k_4}{k_3} (S_{20} + k_3 X_{20} + \frac{k_2}{k_1} S_{10}),$$

$$V_{max} = -\frac{k_4 p_0+p_1^2}{4 q_0} = \frac{1}{4} \frac{k_4}{k_3} \left(C + \frac{k_2}{k_1} a \right)^2 \frac{U_{m2}}{K_{S2}}, \tag{39}$$

$$\lambda = \frac{2-\log(E_1)}{p_0+p_1} = \frac{1}{p_0+p_1} \left[2 - \log \left(\frac{p_0+p_1}{q_0} \frac{(1+A_1)^{\frac{p_1}{c_1}}}{X_{20}} - 1 \right) \right].$$

Thus, the proposed approach relates the parameters of the logistic function (A, V_{max} , and λ) with those of AM2 model.

Identification of AM2 Parameters from Logistic $X_1(t)$ Profile

From the possible estimation of parameters (a_i, b_i , and c_i) and (a_2, b_2 , and c_2) or (A_m, B_m , and C_m) from the logistic functions, and, assuming for instance that the coefficients k_i and K_{Si} are determined by any other means, therefore, by inverting Eq. (37), one can estimate the initial conditions concerning the bacteria's and the substrate (X_{20} and S_{20}) in the bioreactor as well as the parameter of growth rate (U_{m2}) such as:

$$X_{20} = \frac{1}{k_4} \frac{a_2}{1+b_2} (1 + b_1)^{\frac{k_2 V_2}{k_1 V_1}},$$

$$S_{20} = -k_2 \frac{a_1 b_1}{1+b_1} + \frac{k_3}{k_4} \frac{a_2}{1+b_2} (1 + b_1)^{\frac{k_2 V_2}{k_1 V_1}}, \tag{40}$$

$$u_{m2} = \frac{k_4}{k_3} K_{S2} \frac{c_2}{c_1},$$

with $V_1 = \frac{u_{m1}}{K_{S1}} = \frac{(K_{S1}+k_1 a_1) c_1}{K_{S1} k_1 a_1}$ and $V_2 = \frac{u_{m2}}{K_{S2}} = \frac{k_4 c_2}{k_3 a_2}$.

As a conclusion, Eq. (18) and particularly Eq. (33) as well as their inversion establish a link between experimental profile and AM2 model. The presented graphical representations show that the approximation of AM2 model by a logical function is qualitatively relevant. The logistic function profile still follow to some extent AM2 model profile and closer concerning the three characteristic points, which determine the experimental parameters (a_i, b_i , and c_i) and (a_2, b_2 , and c_2) or (A_m, B_m , and C_m). If we consider Eq. (39), they reveal the influence of AM2 parameters and their interaction on the experimental profile by means of the experimental parameters (A, V_{max} , and λ). This relations can be added to the strategies of identification and estimation of AM2 parameters.

CONCLUSIONS

The anaerobic digestion technology is mentioned by the United Nations in the policy of the management of organic wastes among technologies that contribute to achieving sustainable development goals in the future. Considering the importance of this technology, we have performed a comparative and critical analysis of the literature concerning the dynamic models for estimating and predicting the methane production generated by anaerobic bioreactors. We have noticed the lack for single expressions enabling to estimate the evolution of methane production in anaerobic bioreactors but holding significant parameters related to at least two biologic processes that are the acidogenesis and methanogenesis activities such as in AM2 model. There is also

a need to determine these parameters based on the evolution empirical profile of the acidogenic and methanogen bacteria's populations as well as the methane production.

To this end, we have exploited a previous work that has proposed some expressions derived from AM2 model and that meet the profile of the logistic functions for describing the dynamic behavior of the acidogenic and methanogen bacteria's populations as well as the cumulative methane production in batch bioreactors. Therefore, by comparing the parameters of the empirical logistic functions with the logistic functions derived from AM2 model; an estimation of AM2 parameters can be obtained from the empiric profiles of the temporal evolution of acidogenic and methanogen bacteria's populations as well as the cumulative methane production in batch bioreactors and vice versa.

The established relationships lead to more insight in the processes of methane production by enabling the simulation of the influence of most parameters on the cumulated methane production.

A validation of the obtained results has been performed through simulation with graphical representation by comparing the logistic function derived from AM2 model with AM2 itself.

One relevant future work will concern how to exploit the established relations for enhancing the strategies for parameters identification and optimization of methane production in anaerobic bioreactors.

Funding: No funding source is reported for this study.

Acknowledgments: The author would like to thank Scilab software of INRIA for making it freely available to compute, simulate, & draw graphics.

Ethical statement: The author stated that the study did not require ethics committee approval since it did not involve any live subjects. The highest ethical principles were followed during this study.

Declaration of interest: No conflict of interest is declared by the author.

Data sharing statement: Data supporting the findings and conclusions are available upon request from the author.

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