

# Determination of Logistic Model Parameters From AM2 Model for Methane Production for Batch Bioreactors

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## ABSTRACT

Modeling the estimation of cumulated methane production generated from batch anaerobic bioreactors is of paramount importance. In this context, there are two main modeling approaches. The first approach is based on developing mathematical expressions representing the processes involved in the bioreactors. The AM1 model is known as the most complete one. However, it is a complicated model as it requires about 80 parameters to be tuned. A model named AM2 which is a simplified version of AM1 has also been developed. It is based on only two microbial growth processes and requires only 13 parameters. Nevertheless, both AM1 and AM2 models do not provide explicit mathematical expressions that enable to estimate the temporal evolution of methane production with respect to the parameters involved in the considered models. These models are much more useful for simulations and graphical visualizations of the dynamical behavior of the state variables including methane production. On the other hand, the second approach suggests semi-empirical or data-driven models which are based on simple explicit mathematical expressions that provide an estimate of the cumulated methane production (Logistic model, Gompertz model, etc.). But, this type of models require the identification of few parameters which are extracted from experimental data. Usually, they are simplistic and use only one growth process and thus cannot exhibit the influence of the many parameters involved in such complex dynamic biotechnological systems.

In this paper, to overcome the complexity of the first type of models and to avoid the dependency on experimental data in the second type; an explicit analytical mathematical expression is proposed for estimating the cumulated methane production for batch anaerobic bioreactors. This analytical expression is derived via the adoption of some appropriate approximations performed on the set of differential equations characterizing the AM2 model. Therefore, the proposed analytical expression can be considered as an approximation of the AM2 model itself and this is the first contribution of this paper. Graphical profiles of the cumulated methane production are presented showing that of the proposed logistic expression and that of the AM2 model considered as a reference. To the best of the author's knowledge, no such approach and result have been encountered in the literature.

On the other hand, this expression resembles formally to the semi-empirical logistic model. However, the equivalent parameters of the proposed expression as self-defined by the parameters of the AM2 model and do not require experimental data to be identified as it is for the semi-empirical logistic model. Moreover, by comparing the proposed logistic model to the semi-empirical logistic model, an identification of the parameters of the semi-empirical model is linked to the parameters of the AM2 model, providing more insight into the methane production. This can be considered as a second contribution of this paper.

**Keywords:** methane production, anaerobic digestion, logistic model, AM2 model, kinetic models

## INTRODUCTION

Since the beginning of the 21st century, sustainable development is considered as more and more affected by the climate change. One severe factor that influences negatively the environment and the climate change is the misuse of energy generation policy which is responsible of the emission of large amounts of greenhouse gas caused by the combustion

of conventional fossil fuels. Nowadays, it is firmly admitted that renewable energy sources have the potential to reduce emissions of greenhouse gas when replacing fossil fuels and thereby to mitigate climate change. In this context, bioenergy systems can contribute to climate change mitigation if they replace traditional fossil fuel use (Pawlita-Posmik et al., 2018; Sawin and Sverrisson, 2016).

Biogas can be produced by anaerobic digestion of almost every wet organic feedstock such as animal waste, crop

residues, domestic food, industrial wastewater, municipal sewage sludge, etc. Biogas production has been growing steadily in recent years and has made its contribution to renewable energy generation. As a consequence, it reduced negative impacts on the environment, both in the form of greenhouse gas emissions and the pollution of soil and water courses (Wellinger et al., 2013). Anaerobic digestion and biogas technologies contribute also through the reduction of harmful methane emissions from food and farming wastes, providing energy and food security, improving waste management and sanitation, and reducing poverty and hunger (Jain, 2016; Baeyens, Appels, Peng and Dewil, 2016; Wall, Dumont and Murphy, 2018). Moreover, methane gas is also an option for storage of renewable power. It is much easier to handle and safer than hydrogen gas. Many techniques and optimization methods are used to improve the efficiency of anaerobic bioreactors in regard to the expected outputs: gaz production, purification of water and digestates (Mutz, Hengevoss, Hugi and Gross, 2017). The use of membrane in bioreactors for wastewater treatment is a technology that is recently gaining more importance (Sepehri and Sarrafzadeh, 2018).

Thereby, it is worth to have means for predicting and evaluating the methane production produced by anaerobic bioreactors. In this field of research, there are two main approaches (Noll and Henke, 2020).

The first approach is based on mathematical expressions representing the processes involved in the bioreactors. The earlier mathematical models of anaerobic bioreactors have been proposed in the 1970s (Noykova et al., 2002; Yu et al., 2013; Zaher et al., 2009). Depending on the number of biochemical processes considered, there are more or less complex models that have been proposed. The ADM1 model (Anaerobic Digestion Model No. 1) is the most complete model to simulate anaerobic reactors which takes into account most processes involved in bioreactors (Ozgun, 2019; Vavilin et al., 2000). However, this model is very complex because it includes biochemical and physicochemical processes and requires more than 80 parameters to be tuned. The need for more practical models has led to develop the AM2 model which can be considered as a light version of ADM1. It corresponds to the process of anaerobic digestion involving only two phases. Many authors have used AM2 model to study batch and continuous anaerobic digesters with different substrates in various conditions (Noykova et al., 2002; Vavilin, 2000; Zaher et al., 2009). From a mathematical point of view, the AM2 model corresponds to a set of coupled ordinary differential equations of the first order with nonlinear left-hand sides. Because of this nonlinearity, direct analytical solutions about state variables are not easy to determine. Therefore, the solutions are mainly obtained numerically for simulating and visualizing graphically the evolution of the state variables.

Nevertheless, both AM1 and AM2 models do not provide explicit mathematical expressions that enable to estimate the temporal evolution of methane production with respect to the parameters and initial conditions of the considered processes. These models are much more useful for simulations and visualizations of the dynamical behavior of the state variables. In addition, the prediction of methane production in anaerobic reactors by means of mathematical models such as AM1 and

AM2 can have difficulties to fit the experimental measures because of process complexity and sensitivity to the parameters and conditions of experiments.

For these reasons, many empirical or data-driven models have been developed constituting a second approach. They attempt to approximate the methane production by proposing simple formulas to capture the dynamical profile of the methane production. They have adopted various methods: enzymatic, chemical, kinetics, statistical and microbiological growth (Ali et al., 2018; Dewil et al., 2011; Dittmer et al., 2021; Simonov, 2009; Zhang, 2020; Zwiensituting et al., 1990). These models attempt to provide an accurate estimate of the cumulated methane production. One can cite the Transfer Function, Logistic function, Gompertz function, etc which contain some parameters that require identification and adjustment based on experimental data analysis (Parra-Orobio et al., 2017). Usually, this type of models use only one equivalent growth process which is too simplistic and cannot reflect the influence of the many parameters involved in such complex dynamical systems. Among many models, the logistic one is largely used for methane production in anaerobic bioreactors. It provides a mathematical expression that is used for cumulated methane prediction. It requires identification by experimental data analysis of three parameters which have not necessarily biological meanings. The logistic expression has been artificially modified in order to give biological meanings to its three parameters (Crescenzo and Paraggio, 2019; Gerber and Span, 2008; Lemon et al., 2006; Pererva et al., 2020; Van et al., 2018).

This paper intends to present essentially two main contributions.

The first one consists of proposing an explicit analytical mathematical expression for estimating the dynamical cumulated methane production for batch anaerobic bioreactors. This expression is derived via some appropriate approximations applied on the set of differential equations which are characterizing the AM2 model. This explicit function is in the form of a logistic one and depends on the parameters of the AM2 model. Thus, it can be considered as an approximation of the AM2 model for estimating the cumulated methane production. A graphical illustration of both the cumulated methane production obtained by simulation of the AM2 model and of the proposed explicit logistic function is presented enabling to evaluate qualitatively and quantitatively the approximations adopted. The result obtained by simulation is considered as a reference curve.

The second contribution comes from the fact that the proposed function resembles formally to the empiric logistic model which requires the experimental identification of 3 parameters. Thus, by comparing the parameters of the empiric logistic model and its modified version to the proposed one, a link is established between their parameters. Thus, the parameters which have to be identified via experimental data can be expressed in terms of the AM2 model parameters. This approach bridges the AM2 model with both the empirical and the theoretical logistic function ones providing more insight to the methane production.

To the best of the author's knowledge, no such approach or similar results have been encountered in literature concerning

**Table 1.** Parameter values of the two phases processes

$\mu_{1m}$	$K_{S1}$	$\mu_{2m}$	$K_{S2}$	$K_{I2}$	$k_1$	$k_2$	$k_3$	$k_4$
0.4/day	72g/l	0.4/day	18 g/l	103 g/l	13	12	22	75

the estimation of cumulated methane production of batch anaerobic bioreactors. As a consequence, this proposed logistic function enables to overcome the complexity of the first type of models as well as the dependency on experimental data in the second type of models.

The paper is organized as follows: First section gives an introduction about the issue under consideration. The second section presents the AM2 model. The third section determines the concentration of the acidogenic bacteria population  $X_1(t)$  which is required in order to determine the concentration of the methanogenic bacterial population  $X_2(t)$ . Section four establishes the general solution of  $X_2(t)$  and its particular solution given an exponential approximation of  $X_1(t)$ . Section five reveals the formal resemblance between the logistic function and the inferred expression  $X_2(t)$  that leads to predict the cumulated methane production. Last section concludes the paper.

## EQUATIONS GOVERNING THE AM2 MODEL

The mathematical AM2 model is based on the laws of growth (Simonov et al., 2009). It involves the following dynamic variables:  $X_1$  is the concentration of the acidogenic bacteria population;  $X_2$  is the concentration of the methanogenic bacterial population;  $S_1$  is the concentration of the substrate of carbonaceous material and  $S_2$  is the substrate concentration of volatile fatty acids. For batch systems, the mathematical model is expressed in the form of a coupled differential equations of the first order system:

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

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

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

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

For the growth process, the function of Monod  $\mu_1$  for acidogens bacteria and the function of Haldane  $\mu_2$  for methanogens bacteria are respectively:

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

with  $\mu_{1m}$  the maximal growth rate and  $K_{S1}$  the constant of half-saturation, and

$$\mu_2 = \mu_{2m} \frac{S_2}{S_2 + \frac{S_2^2}{K_{I2}} + K_{S2}} \quad (6)$$

with  $\mu_{2m}$  the maximal growth rate,  $K_{S2}$  the constant of saturation and  $K_{I2}$ , the constant of inhibition.

The flow of methane which is the end product depends directly on the growth of methanogenic bacteria population  $X_2$ , according to the relation:

**Table 2.** Initial conditions values

$S_1(0)$	$S_2(0)$	$X_1(0)$	$X_2(0)$
10 g/l	2 g/l	0.4 g/l	0.01 g/l

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

The cumulative quantity  $C(t)$  of the produced methane can be estimated by:

$$C(t) = k_4 \cdot X_2(t) \quad (8)$$

For the implementation, this model can be written in a state space form such as:

$$\frac{dz(t)}{dt} = f(z(t)) \quad (9)$$

with the state space vector:

$$z(t) = (X_1(t) \quad X_2(t) \quad S_1(t) \quad S_2(t))^T$$

and initial conditions:

$$z(t_0) = (X_1(t_0) \quad X_2(t_0) \quad S_1(t_0) \quad S_2(t_0))^T$$

There are nine parameters involved in this model ( $\mu_{1m}$ ,  $K_{S1}$ ,  $\mu_{2m}$ ,  $K_{S2}$ ,  $K_{I2}$ ,  $k_1$ ,  $k_2$ ,  $k_3$ ,  $k_4$ ). To solve mathematically this system of differential equations, we must also provide four initial conditions:  $S_1(0)$ ,  $S_2(0)$ ,  $X_1(0)$  and  $X_2(0)$ .

This ODE system has been implemented by means of Euler's integration method and also has been solved by using the ODE function of Scilab software. The graphical results obtained by solving this system correspond to a simulation carried out with the following parameter values of the two phases processes (Table 1).

The initial condition values are shown in Table 2.

## ANALYTICAL APPROACH FOR $S_1(t)$ AND $X_1(t)$

### Temporal Evolution of Substrate $S_1(t)$

To analyze the system of differential equations of AM2 model, consider the differential equations  $X_1(t)$  et  $S_1(t)$  corresponding to equations (1) and (3). It can be noticed that they are in fact decoupled from equations  $X_2(t)$  and  $S_2(t)$ . Therefore, by combining (1) and (3), one can write the following equalities:

$$\frac{dS_1}{dt} = -k_1 \cdot \mu_1 \cdot X_1(t) = -k_1 \cdot \frac{dX_1}{dt} \quad (10)$$

by integrating (10), one gets the following linear relationship between  $S_1(t)$  and  $X_1(t)$  that is:

$$S_1 = -k_1 \cdot X_1(t) + S_{10} + k_1 \cdot X_{10} \quad (11)$$

where  $X_{10}$  and  $S_{10}$  are respectively the initial values of  $X_1(t)$  and  $S_1(t)$ .

To explicit  $X_1(t)$ , let's replace  $\mu_1$  in (10) by its expression in (1) so that one gets the relation:

$$\frac{dS_1}{dt} = -k_1 \cdot \mu_1 \cdot X_1 = -k_1 \cdot \mu_{1m} \cdot \frac{S_1}{(S_1 + K_{S1})} \cdot X_1 \quad (12)$$

replacing  $X_1(t)$  by its expression obtained in (11), one gets the following first order non linear differential equation in terms of  $S_1(t)$  with respect to the time independent variable:

$$\frac{dS_1}{dt} = \mu_{1m} \cdot \frac{S_1}{(S_1 + K_{S1})} \cdot (S_1 - \alpha) \tag{13}$$

with:  $\alpha = S_{10} + k_1 \cdot X_{10}$

By separating the variables from both sides in (13), it can be rewritten in the following form:

$$\frac{(S_1 + K_{S1})}{S_1 \cdot (S_1 - \alpha)} \cdot \frac{dS_1}{dt} = \mu_{1m} \tag{14}$$

By introducing the initial conditions, one obtains the solution of (14) in an analytical inverse form  $t=f(S_1)$ :

$$t = f(S_1) = \frac{(K_{S1} + \alpha)}{\alpha \cdot \mu_{1m}} \cdot \ln\left(\frac{|S_1 - \alpha|}{|S_{10} - \alpha|}\right) - \frac{K_{S1}}{\alpha \cdot \mu_{1m}} \cdot \ln\left(\frac{S_1}{S_{10}}\right) \tag{15}$$

It is not possible to express  $S_1(t)$  in a standard form. So, from (15),  $S_1(t)$  can be easily computed and graphically represented by only generating values to  $S_1$  and computing consequently the corresponding time  $t$ .

**Temporal Evolution of Bacteria  $X_1(t)$**

The dynamic evolution of bacteria  $X_1(t)$  can be derived from relation (11) as follows:

$$X_1(t) = -\frac{1}{k_1} (S_1(t) - a) \tag{16}$$

Similarity to  $S_1(t)$ ,  $X_1(t)$  cannot be expressed in a direct analytical standard form but can be expressed in the inverse form:  $t=g(X_1)$  as follows:

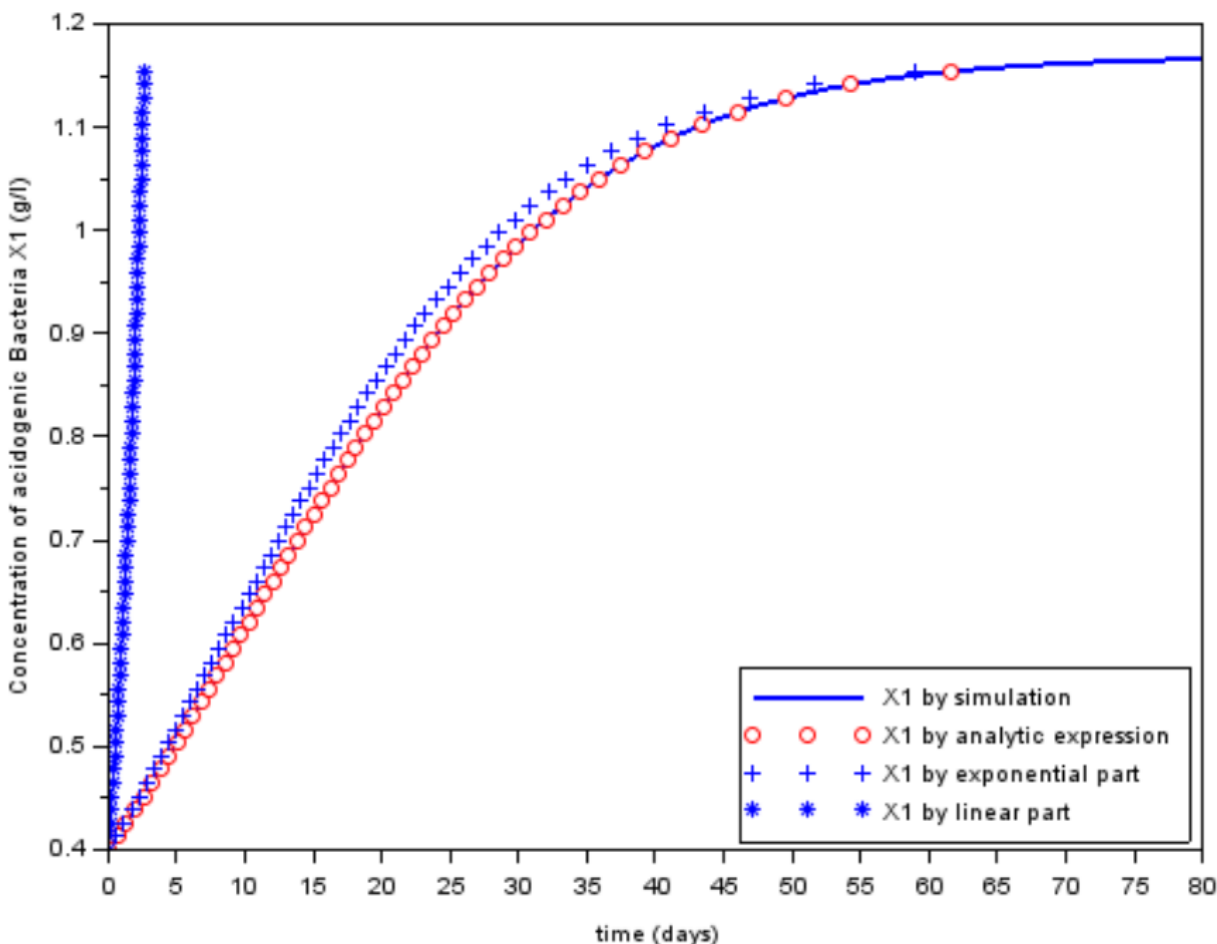
$$t = \frac{K_{S1}}{\alpha \cdot \mu_{1m}} \cdot \ln\left(\frac{|X_1(t)|}{X_{10}}\right) - \frac{K_{S1}}{\alpha \cdot \mu_{1m}} \cdot \ln\left(\frac{|k_1 \cdot X_1(t) - \alpha|}{|k_1 \cdot X_{10} - \alpha|}\right) + \frac{1}{\mu_{1m}} \cdot \ln\left(\frac{|X_1(t)|}{X_{10}}\right) \tag{17}$$

The analytical expressions (15) and (17) include the model parameters ( $K_{S1}$ ,  $\mu_{1m}$ ,  $k_1$ ) and the initial values ( $S_{10}$ ,  $X_{10}$ ). They enable to analyze the evolution of  $S_1(t)$  and  $X_1(t)$  as well as their sensitivity to the related model parameters. By varying the values of  $X_1(t)$ , the values of the corresponding time are computed and the function  $X_1=g^{-1}(t)$  can be drawn. Graphics of  $X_1(t)$  obtained by numerical simulation from the AM2 model (blue segments) and also from the analytical expression (17) (red circles) as implemented under Scilab software are presented in **Figure 1**. They appear superimposed and thus are similar.

Moreover, in order to obtain an approximate analytical expression of  $X_1(t)$  derived from (17), one needs to examine this expression which is composed of three parts. A graphical representation of the parts composing (17) can reveal the combination that can provide the best approximation of  $X_1(t)$ . Let's consider the first part of (17) that is constituted of the following expression:

$$t_a = \frac{(K_{S1})}{\alpha \cdot \mu_{1m}} \cdot \ln\left(\frac{|X_1(t)|}{X_{10}}\right) - \frac{K_{S1}}{\alpha \cdot \mu_{1m}} \cdot \ln\left(\frac{|k_1 \cdot X_1(t) - \alpha|}{|k_1 \cdot X_{10} - \alpha|}\right) \tag{17-a}$$

This expression (17-a) is represented graphically by the blue + in **Figure 1**. This curve is very close to the theoretical curve drawn from (17) with red circles. The profiles of these two curves are almost exponential, therefore, (17-a) can be



**Figure 1.** Analytical expression of  $X_1(t)$  and its approximation

considered as an approximate expression of (17). The second part of expression (17) that is left is:

$$t_b = \frac{1}{\mu_{1m}} \cdot \ln\left(\left|\frac{X_1(t)}{X_{10}}\right|\right) \quad (17-b)$$

It corresponds to the curve that is approximately a line (in blue star) situated at the left side of **Figure 1** and which can be neglected.

### Some Remarks

#### Behavior evolution of $S_1(t)$ and $X_1(t)$

Although the equation of  $X_1(t)$  and  $S_1(t)$  are non-linear, there profiles present behaviors like systems whose dynamics are characterized by a transient response followed by a steady state response. So, to determine the steady state asymptotic value of  $X_1(t)$  which is reached for large time values, it requires combining (3), (5), (11) and equaling to zero the first derivative of  $X_1(t)$ :

$$\frac{dX_1}{dt} = \mu_{1m} \cdot \frac{S_1}{(S_1 + K_{S1})} \cdot X_1 = \mu_{1m} \cdot \frac{(-k_1 \cdot X_1 + \alpha) \cdot X_1}{(-k_1 \cdot X_1 + K_{S1} + \alpha)} = 0$$

This leads to the condition:  $-k_1 \cdot X_1 + \alpha = 0$ , which consequently leads to the asymptotic steady state value of acidogenic bacteria:  $X_1(t) = X_{1S} = \frac{\alpha}{k_1} = X_{10} + \frac{S_{10}}{k_1} \cong 1.17 \text{ g/l}$ . Similarly, from equation (11), we can determine the asymptotic steady state value for  $S_1(t)$  which tends to zero. This means that the concentration of the substrate of carbonaceous material will be almost completely consumed at relatively large time durations.

#### Settling time for $X_1(t)$ and $S_1(t)$

In such systems, it is important to determine the settling time  $t_{set}$  which is defined as the time to reach the steady state value up to 5%. For  $X_1(t)$ , it corresponds to:

$$X_1(t_{set}) = X_{1set} = 0.95 \cdot X_{1S} = 1.11 \text{ g/l}$$

By replacing this settling value  $X_{1set}$  in (12), the settling time  $t_s$  is about 45 days. From equation (11), we can estimate the settling value for  $S_1(t)$  which is about 50 days. The comparison of these results are in full agreement with those given by simulation of the system of differential equations composing AM2 model.

## TEMPORAL EVOLUTION OF $X_2(t)$

#### Establishment of Differential Equations for $X_2(t)$

From the previous equations (2) and (4), we can write:

$$\frac{dX_2}{dt} = \mu_2 \cdot X_2 = \mu_{2m} \cdot \frac{S_2}{S_2 + \frac{S_2^2}{K_{S2}} + K_{S2}} \cdot X_2 \quad (18)$$

On the other hand, by using (1) and (2), equation (4) can be written in the following form:

$$\frac{dS_2}{dt} = k_2 \frac{dX_1}{dt} - k_3 \frac{dX_2}{dt} \quad (19)$$

by integrating this last equation (19), we obtain:

$$S_2(t) = k_2 X_1(t) - k_3 \cdot X_2(t) + C \quad (20)$$

which can also be written as:

$$S_2(t) = -k_3 X_2(t) + k_2 \cdot X_1(t) + C = -k_3 \cdot X_2 + f(t) \quad (21)$$

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

By replacing  $S_2(t)$  from (21) into the (18), we can explicit a nonlinear differential equation of the first order on  $X_2(t)$  which depends on  $X_1(t)$  via the term  $b(t)$ :

$$\frac{dX_2}{dt} = \mu_{2m} \cdot \frac{(-k_3 \cdot X_2 + f) \cdot X_2}{[(-k_3 \cdot X_2 + f) + \frac{(-k_3 \cdot X_2 + f)^2}{K_{S2}} + K_{S2}]} = g(X_2, X_1) \quad (22)$$

Under this form, the differential equation (22) cannot be solved to obtain an analytical expression. This is only possible in the case where  $X_1(t)$  is independent from time which is not the case in our general problem since we know already the profile of  $X_1(t)$  as given by (17).

#### Approximation of the Growth Process of Bacteria $\mu_2(S_2)$

To obtain analytical solutions for  $X_2(t)$  and  $S_2(t)$ , it is necessary to make some approximations that simplify the differential equations (21) and (22). That is the only way to make them amenable to expressions that are analytically integrable. To be solvable analytically, it needs again to be simplified to the level that the growth law of the methanogenic process of the bacterial population becomes linear of the form:

$$\mu_2 = \frac{\mu_{2m}}{K_{S2}} \cdot S_2 \quad (23)$$

By adopting these simplifications, (22) can be written as follows:

$$\begin{aligned} \frac{dX_2}{dt} &= \mu_{2m} \cdot \frac{S_2}{K_{S2}} \cdot X_2 = \mu_{2m} \cdot \frac{(-k_3 \cdot X_2 + k_2 \cdot X_1 + C) \cdot X_2}{K_{S2}} \\ &= \mu_{2m} \cdot \frac{f(t) \cdot X_2 - k_3 \cdot X_2^2}{K_{S2}} \end{aligned} \quad (24)$$

Now, the differential equation (24) corresponds to Bernoulli's differential equation [Parker, 2020]. It can be rewritten to match the standard form of Bernoulli's differential equation for the particular case where the coefficient  $n=2$ ; that is:

$$\frac{dy(t)}{dt} + P(t) \cdot y(t) = Q(t) \cdot y^2(t) \quad (25)$$

Therefore, equation (24) structured in the standard Bernoulli's form becomes:

$$\frac{dX_2(t)}{dt} - \frac{\mu_{2m}}{K_{S2}} (C + k_2 \cdot X_1(t)) \cdot X_2(t) = -\frac{\mu_{2m}}{K_{S2}} \cdot k_3 \cdot X_2^2(t) \quad (26)$$

with

$$P(t) = -\frac{\mu_{2m}}{K_{S2}} (C + k_2 \cdot X_1(t)) \quad (27)$$

And

$$Q(t) = q_0 = -\frac{\mu_{2m}}{K_{S2}} \cdot k_3 \quad (28)$$

To solve (25), it is converted into another simpler differential equation of the first order that has a general solution (Parker, 2020):

$$y(t) = \frac{e^{-\int_0^t P(t) \cdot dt}}{c_0 - \int_0^t Q(t) \cdot e^{-\int_0^t P(t) \cdot dt} \cdot dt} \quad (29)$$

To explicit the general solution in the form of (29), it requires the provision of  $P(t)$  which means to provide the profile of  $X_1(t)$ . Here again, the problem of integrating this function is not obvious in standard analytical expressions. So, in this paper, we will use an exponential approximation for  $X_1(t)$  as announced earlier.

### Exponential Approximation of $X_1(t)$

We approximate  $X_1(t)$  by the exponential part expressed by (17-a) that is:

$$t \approx -\frac{K_{s1}}{\alpha \cdot u_{1m}} \cdot \ln\left(\left|\frac{X_{10}}{X_1(t)}\right| \left|\frac{k_1 \cdot X_1(t) - \alpha}{k_1 \cdot X_{10} - \alpha}\right|\right)$$

The exponential approximation of  $X_1(t)$  can be written in a form that corresponds to a Logistic Function as follows:

$$X_{1e}(t) = \frac{\alpha}{k_1} \cdot \left(\frac{1}{1 + A_1 \cdot \exp(-\frac{t}{B})}\right) \quad (30)$$

with

$$B = \frac{K_{s1}}{\alpha \cdot u_{1m}}; \quad A_1 = \frac{S_{10}}{k_1 \cdot X_{10}}$$

### Determination of $X_2(t)$ with Exponential Approximation of $X_1(t)$

To explicit  $X_2(t)$  from (29) given the exponential approximation of  $X_1(t)$ , we need to define the functions  $P_e(t)$  and  $Q_e(t)$  respectively from (26) and (27). In expression (26), we replace  $X_1(t)$  par the exponential approximation as follows:

$$P_e(t) \equiv -\frac{\mu_{2m}}{K_{s2}} (C + k_2 \cdot X_{1e}(t))$$

it can be written in the form:

$$P_e(t) = -\frac{\mu_{2m}}{K_{s2}} \cdot C - \frac{\mu_{2m} \cdot k_2 \cdot a}{k_{s2} \cdot k_1} \cdot \left(\frac{1}{1 + A_1 \cdot \exp(-t/B)}\right) \quad (31)$$

$$= p_{0e} + p_{1e} \cdot \frac{1}{(1 + A_1 \cdot \exp(-t/B))}$$

with

$$p_{0e} = -\frac{\mu_{2m}}{K_{s2}} C$$

$$p_{1e} = -\frac{\mu_{2m}}{K_{s2}} k_2 \cdot \frac{a}{k_1} = -\frac{\mu_{2m}}{K_{s2}} \cdot \frac{k_2}{k_1} \cdot (S_{10} + k_1 \cdot X_{10})$$

$Q(t)$  becomes  $Q_e(t)$ :

$$Q_e(t) = q_0 = -\frac{\mu_{2m}}{K_{s2}} \cdot k_3$$

Now, we can determine  $X_2(t)$  from expression (29). The integral at the numerator can be computed:

$$I(t) = \int_0^t P_e(t) \cdot dt = p_{0e} \cdot t + p_{1e} \cdot B \cdot \ln(A_1 + \exp(\frac{t}{B})) \quad (31-a)$$

$$- p_{1e} \cdot B \cdot \ln(A_1 + 1)$$

With some basic transformations, this expression can be written :

$$I(t) = p_{0e} \cdot t + p_{1e} \cdot B \cdot \ln\left[\exp(\frac{t}{B}) \cdot (1 + A_1 \cdot \exp(-\frac{t}{B}))\right] \quad (31-b)$$

$$- p_{1e} \cdot B \cdot \ln(1 + A_1)$$

and:

$$I(t) = -p_{1e} \cdot B \cdot \ln(1 + A_1) + (p_{0e} + p_{1e}) \cdot t \quad (31-c)$$

$$+ p_{1e} \cdot B \cdot \ln\left[1 + A_1 \cdot \exp(-\frac{t}{B})\right]$$

The expression of the numerator is:

$$N(t) = \exp\left[-\int_0^t P_e(t) \cdot dt\right] = \exp[p_{1e} \cdot B \cdot \ln(1 + A_1) - (p_{0e} + p_{1e}) \cdot t] \quad (32)$$

$$- p_{1e} \cdot B \cdot \ln\left(1 + A_1 \cdot \exp(-\frac{t}{B})\right)$$

The denominator can be expressed as follows:

$$D(t) = c_0 - q_0 \cdot \int_0^t e^{N(t)} \cdot dt \quad (33)$$

$$= c_0 - q_0 \cdot \int_0^t \exp[(p_{1e} \cdot B \cdot \ln(1 + A_1)) - (p_{0e} + p_{1e}) \cdot t - p_{1e} \cdot B \cdot \ln(1 + A_1 \cdot \exp(-\frac{t}{B}))] \cdot dt$$

By taking into account the initial value of  $X_2(0) = X_{20}$ ; it gives:  $c_0 = 1/X_{20}$ . Finally, the expression  $X_{2e}(t)$  can be written as follows:

$$X_{2e}(t) = \frac{x_{20} \cdot \exp[p_{1e} \cdot B \cdot \ln(1 + A_1) - (p_{0e} + p_{1e}) \cdot t - p_{1e} \cdot B \cdot \ln(1 + A_1 \cdot \exp(-t/B))]}{1 - x_{20} \cdot q_0 \cdot \int_0^t \exp[(p_{1e} \cdot B \cdot \ln(1 + A_1) - (p_{0e} + p_{1e}) \cdot t - p_{1e} \cdot B \cdot \ln(1 + A_1 \cdot \exp(-t/B)))] \cdot dt} \quad (34)$$

In this last expression (34), the parameters ( $p_{0e}$ ,  $p_{1e}$ ,  $q_0$ ,  $B$ ) depend from the parameters of the AM2 model. Then,  $X_{2e}(t)$  will depend on the values of these parameters. However, the integral on the denominator cannot be written in standard forms but can only be expressed with special functions such as the error function  $\text{erf}(x)$ , the incomplete gamma function  $\gamma(x, z)$  and exponential integral function  $\text{Ei}(x)$ . It is thus difficult to analyze  $X_{2e}(t)$  including these special functions.

### Determination of $X_2(t)$ with Exponential Approximation of $X_1(t)$

It is difficult to analyze  $X_{2e}(t)$  with these special functions. For this reason, in order to overcome these difficulties, we will consider an approximation that simplifies the expression (34). To this end, we will neglect the parts that vanishes for relatively large values of  $t$  that correspond to the steady state response.

so, consider the numerator (32), for relatively large  $t$ , the term  $p_{1e} \cdot B \cdot \exp(-t/B)$  tends to vanish in the numerator and in the denominator. Therefore, the expression  $N_e(t)$  becomes:

$$N_e(t) \cong \exp\left[-\int_0^t P_e(t) \cdot dt\right] = \exp[p_{1e} \cdot B \cdot \ln(1 + A_1) - (p_{0e} + p_{1e}) \cdot t] \quad (35)$$

$$N_e(t) \cong (1 + A_1)^{p_{1e} \cdot B} \cdot \exp(-p_{0e} - p_{1e}) \cdot t$$

with this approximation  $D_e(t)$  becomes integrable and is:

$$D_e(t) \cong 1 - x_{20} \cdot q_0 \cdot \int_0^t e^{N_e(t)} \cdot dt \quad (36)$$

$$= 1 - x_{20} \cdot \frac{q_0}{(p_{0e} + p_{1e})} \cdot (1 + A_1)^{p_{1e} \cdot B} \cdot [1 - \exp(-p_{0e} - p_{1e}) \cdot t]$$

replacing this new results in (29) or (34), we obtain the final expression:

$$X_{2e}(t) \cong \frac{x_{20} \cdot (1 + A_1)^{p_{1e} \cdot B} \cdot \exp(-p_{0e} - p_{1e}) \cdot t}{1 - \frac{q_0}{(p_{0e} + p_{1e})} \cdot x_{20} \cdot (1 + A_1)^{p_{1e} \cdot B} [1 - \exp(-p_{0e} - p_{1e}) \cdot t]} \quad (37)$$

which shows that the growth of methanogens bacteria under our approximations can be written in the form of a logistic function with parameters related to the AM2 model:

$$X_{2e}(t) \cong \frac{(p_{0e} + p_{1e})}{q_0} \cdot \frac{1}{(1 + E_1 \cdot \exp(p_{0e} + p_{1e}) \cdot t)} \quad (38)$$

with:

$$E_1 = \frac{E}{D} = \frac{1}{D} - 1 = \frac{(p_{0e} + p_{1e})}{q_0 \cdot x_{20} \cdot (1 + A_1)^{p_{1e} \cdot B}} - 1$$

## PREDICTION OF METHANE PRODUCTION

### Determination of the Parameters of the Logistic Function

To evaluate the cumulated methane production from the AM2 model, we may use the expression (7) and (8). The cumulated quantity of methane over a given period  $t$  is proportional to  $X_2(t)$ .

If we consider our approximation, it can be written as:

$$V_{2e}(t) = k_4 \cdot X_{2e}(t) \cong k_4 \cdot \frac{(p_{0e} + p_{1e})}{q_0} \cdot \left( \frac{1}{1 + E_1 \cdot \exp(p_0 + p_1) \cdot t} \right) \quad (39)$$

where  $k_4$  is the production parameter of methane for the AM2 model.

It can be rewritten after some elementary operations and arranged in the form of a logistic function:

$$V_{2e}(t) = k_4 \cdot X_{2e}(t) \cong k_4 \cdot \frac{(p_{0e} + p_{1e})}{q_0} \cdot \left( \frac{1}{1 + \exp[\ln(E_1) + (p_0 + p_1)t]} \right) \quad (40)$$

The empirical logistic function that is used for predicting the cumulative methane production is usually expressed as follows (Crescenzo and Paraggio., 2019; Gerber and Span., 2018; Lemon et al., 2006).

$$V(t) = \frac{a}{1 + \exp(b + c \cdot t)} \quad (41)$$

where  $V(t)$  is the methane volume in time  $t$  and  $(a, b, c)$  are three parameters that have to be determined via an analysis of a set of experimental data.

The expressions  $V(t)$  in (40) and  $V_{2e}(t)$  in (41) become comparable. By comparing them, we can identify the parameters in both models. The empirical parameters expressed in terms of the approximate AM2 adopted model can be written in the form:

$$a = k_4 \cdot \frac{(p_0 + p_1)}{q_0} = \frac{k_4}{k_3} \cdot \left( \frac{k_2}{k_1} \cdot S_{10} + S_{10} + k_3 \cdot X_{20} \right) \\ b = \log(E_1) = \left[ \ln \left( \frac{(p_0 + p_1)}{q_0} \cdot \frac{(1 + A_1)^{-p_{1B}}}{x_{20}} - 1 \right) \right] \\ c = -(p_0 + p_1)$$

in order to give a meaning to the parameters of the empirical logistic function, it is useful to use its modified version known as the modified logistic function. By some elementary mathematical transformations, the logistic function with  $(a, b, c)$  parameters can be transformed into the modified logistic function and expressed as:

$$Vm(t) = \frac{A}{1 + \exp\left(-\frac{A \cdot v_{max}}{A} (t - \lambda) + 2\right)} \quad (42)$$

In (42),  $Vm(t)$  is the cumulated methane volume at time  $t$ . It requires the determination of three parameters via an analysis of the experimental data. They are: the maximum methane production ( $A$ ) (mL), the duration of the lag phase ( $\lambda$ ) (hours), and the maximum rate of methane production ( $v_{max}$ ) (mL-h<sup>-1</sup>).

To make the approximate AM2 model  $V_{2e}(t)$  comparable to the modified logistic function  $Vm(t)$ , we transform again the expression (40) to resemble (42) as follows:

$$V_{2e}(t) = k_4 \cdot \frac{(p_0 + p_1)}{q_0} \cdot \frac{1}{\left(1 + \exp\left[\left(p_0 + p_1\right) \cdot \left(t - \frac{2 - \log(E_1)}{(p_0 + p_1)}\right) + 2\right]\right)} \quad (43)$$

By comparing (42) with (43), the parameters of the modified logistic function can be expressed in terms of the approximate AM2 model parameters:

$$A = k_4 \cdot \frac{(p_0 + p_1)}{q_0} = \frac{k_4}{k_3} \cdot \left( C + \frac{k_2}{k_1} \cdot a \right) = \frac{k_4}{k_3} \cdot \left( S_{20} + k_3 \cdot X_{20} - k_2 \cdot X_{10} + \frac{k_2}{k_1} \cdot S_{10} \right) \\ v_{max} = \frac{k_4 (p_0 + p_1)^2}{4 q_0} = \frac{1}{4} \frac{\mu_{2m} k_4}{K_{s2} k_3} \left( C + \frac{k_2}{k_1} \cdot a \right)^2 \quad (44) \\ \lambda = \frac{(2 - \log(E_1))}{(p_0 + p_1)} = \frac{1}{(p_0 + p_1)} \left[ 2 - \log\left(\frac{(p_0 + p_1)}{q_0} \cdot \frac{(1 + A_1)^{-p_{1B}}}{x_{20}} - 1\right) \right]$$

We notice that the parameters of the logistic function depend from the parameters of the AM2 model as well as from the initial conditions. Thus, the proposed approach relates the parameters of the logistic function with those of the AM2 model giving a biotechnological sense to them.

The lag time has to be positive, we can impose a condition that is:

$$\lambda = \frac{(2 - \log(E_1))}{(p_0 + p_1)} = \frac{1}{(p_0 + p_1)} \left[ 2 - \log\left(\frac{(p_0 + p_1)}{q_0} \cdot \frac{(1 + A_1)^{-p_{1B}}}{x_{20}} - 1\right) \right] > 0 \quad (45)$$

### Comparison of Profiles AM2 Model to the Proposed Logistic Function

To analyze what the approximations adopted over the AM2 in order to get an analytical expression for the cumulated methane production, we draw the curve obtained by solving numerically the system of AM2 equations. It is the blue curve represented in **Figure 2**. The red curve corresponds to the approximate analytical expression  $V_{2e}(t)$  based on AM2 model.

For relatively large values of  $t$  which correspond to the steady state, these curves converge towards the same asymptotic value that is:

$$V_{2e}(\infty) = k_4 \cdot X_{2e}(\infty) = \frac{k_4 \cdot X_{2S}}{k_3} = \frac{k_4}{k_3} \cdot \left[ \frac{k_2}{k_1} \cdot S_{10} + S_{20} + k_3 \cdot X_{20} \right] \quad (46)$$

## CONCLUSION

A mathematical expression formally comparable to the empirical logistic function is proposed for estimating the cumulative methane production for batch reactors. It is derived through some appropriate approximations performed on the set of differential equations characterizing the AM2 model.

The comparison of the empirical logistic function with the proposed expression enabled to express the three parameters of the empiric logistic function as well as its modified version in terms of the AM2 parameters.

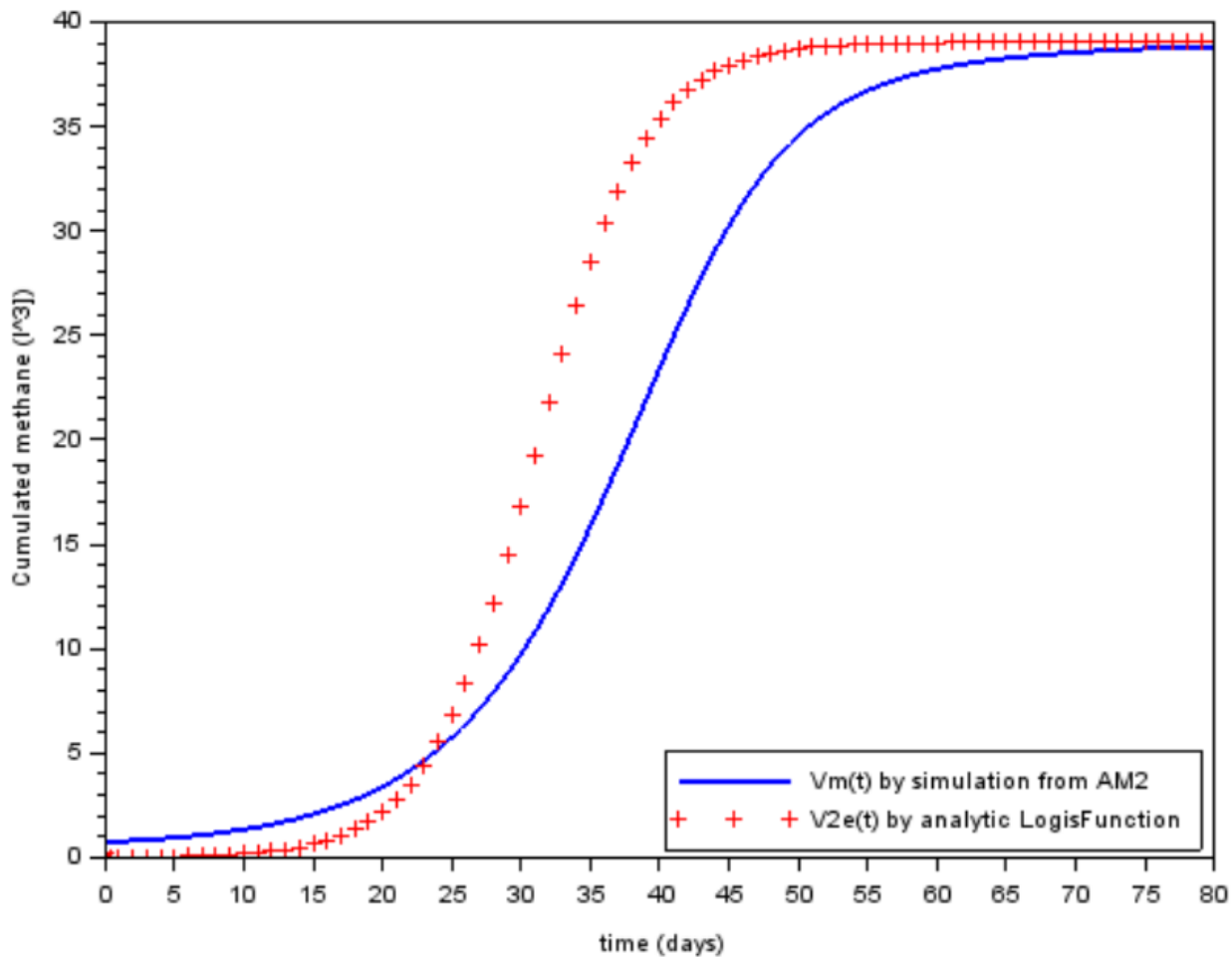


Figure 2. Profile of approximate Logistic function based AM2

The relations between the sets of both parameters reveals the complexity of the methane production processes. This approach bridges the mathematical AM2 model with the empirical one providing more insight in the methane production.

As perspectives, a study has to be carried out in order to analyze the influence of the parameters of the AM2 on the proposed logistic function. This study has also to compare the parameters of the empiric logistic function which are identified experimentally with those obtained by the proposed logistic function.

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