

# AN ANALYTICAL APPROACH TO AM2 MODEL FOR BATCH ANAEROBIC BIOREACTORS

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**Abstract:** *The well-known AM2 model is commonly used for simulation of biotechnological processes of two-phases anaerobic digestions. Nevertheless, numerical simulation and graphical results usually obtained by solving the non-linear system of differential equations characterizing this model do not always enable an easy analysis of the processes as well their sensitivity to the variations of the different parameters and the initial conditions. In this paper, as an alternative to simulation, an analytical approach is proposed for batch reactors. It consists of adopting some approximations to reduce the mathematical complexity of the coupled differential equations of the AM2 model. The aim is to derive approximate analytical expressions concerning the dynamical evolution of the substrates and bacteria involved in reactions. The obtained expressions, therefore, permit a relatively easy analysis of the evolution of the main processes and their sensitivity to the different parameters and initial conditions. Moreover, it provides an explicit mathematical expression that enables to estimate the cumulative production of methane. The comparison of the obtained results by this proposed analytical approach to the numerical simulation of the AM2 model shows a satisfying qualitative convergence of the proposed approach to the AM2 model.*

## 1. INTRODUCTION

A practical mathematical model named AM2 is very useful for simulating and analyzing biological process of anaerobic digestion of two phases. Many authors have used this model to study batch and continuous anaerobic digesters with different substrates in various conditions [1-3]. From the mathematical point of view, the AM2 model corresponds to a set of coupled ordinary differential equations (ODE) of the first order with non linear left hand sides. Because

of this non linearity, explicit analytical solutions about state variables cannot be obtained; so the solutions are only obtained numerically by various numerical integration methods and serve to simulate and visualize graphically the evolution of the state variables. Most of the results obtained by different authors, based on AM2 model, are qualitatively comparable but quantitatively they may differ. Indeed, the results are very sensitive with respect to the change of the parameter values and to the conditions of experiments [4]. This fact expresses the complexity of the phenomenon regarding the limits of this model.

However, while the numerical simulation can graphically present the evolution of the different state variables, it doesn't always enable an easy analysis of the processes as well as the influence of the different parameters involved in the model and the conditions of experiments. In the literature, approaches leading to even approximate solutions of the AM2 model are very few or limited to analyzing the stability of the AM2 model [6]. Most of analytical approaches propose approximate expressions of the output state variable that is usually the production of methane based on simplifications and empirical formulas [5-10].

In this paper, It is intended to solve the AM2 model by using an analytical approach. By adopting some approximations over the equations of the model, this approach led to obtain some analytical expressions concerning the dynamical evolution of the substrates and bacteria during the processes. The obtained analytical expressions enable to have an insight on the complexity of the problem and to perform a detailed analysis of the temporal evolution of the main processes and the influence of the different parameters involved in the mathematical model. The comparison of this analytical approach to the numerical simulation shows qualitatively a satisfying convergence of the former approach and therefore justifies its use within the limits of the adopted approximations.

## 2. EQUATIONS GOVERNING THE AM2 MODEL

### 2.1. Mathematical Formulation

The mathematical AM2 model is based on the laws of growth [4]. 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 adopted and they are respectively:

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

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

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

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  $X_2(t)$ , according to the relation:

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

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

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

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 mathematically solve this system of differential equations, we must also provide four initial conditions:  $S_1(0)$ ,  $S_2(0)$ ,  $X_1(0)$  and  $X_2(0)$ .

## 2.2. State Space Model

The system constituted of the differential equations (1), (2), (3) and (4) is a set of coupled differential equations of first order with non linear functions at the right hand side. Its integration provides the temporal evolution of the bacteria and the substrate concentrations. The production of the methane can be deduced from equation (7) and (8). For the implementation, this model can be written in a state space form such as:

$$\frac{dz(t)}{dt} = f(z(t)) = \begin{pmatrix} X_1(t) \\ X_2(t) \\ S_1(t) \\ S_2(t) \end{pmatrix} = \begin{pmatrix} f_1(z) \\ f_2(z) \\ f_3(z) \\ f_4(z) \end{pmatrix} = \begin{pmatrix} \mu_1 \cdot X_1 \\ \mu_2 \cdot X_2 \\ -k_1 \cdot \mu_1 \cdot X_1 \\ k_2 \cdot \mu_1 \cdot X_1 - k_3 \cdot \mu_2 \cdot X_2 \end{pmatrix} \quad (9)$$

with the state space vector:  $z(t) = (X_1(t) \ X_2(t) \ S_1(t) \ S_2(t))^T$

and initial conditions are:  $z(t_0) = (X_1(t_0) \ X_2(t_0) \ S_1(t_0) \ S_2(t_0))^T$

This ODE system has been implemented by means of Euler's integration method and has been solved by using the ODE function of SCILAB software [11]. The graphical results obtained by solving this system correspond to a simulation carried out with the following parameter values:  $\mu_{1m} = 0.4/\text{day}$ ;  $K_{s1} = 72 \frac{\text{g}}{\text{l}}$ ;  $\mu_{2m} = 0.4/\text{day}$ ;  $K_{s2} = 18 \frac{\text{g}}{\text{l}}$ ;  $K_{I2} = 103 \text{ g/l}$ ;  $k_I = 13$ ;  $k_2 = 12$ ;  $k_3 = 22$ ; and the initial values are:  $S_I(0) = 10 \text{ g/l}$ ;  $S_2(0) = 2 \text{ g/l}$ ;  $X_I(0) = 0.4 \text{ g/l}$  and  $X_2(0) = 0.01 \text{ g/l}$ .

## 3. ANALYTICAL APPROACH FOR $S_I(t)$ AND $X_I(t)$

### 3.1. Temporal evolution of substrate $S_I(t)$

To analyze the system of differential equations of AM2 model, consider the differential equations  $X_I(t)$  and  $S_I(t)$  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), it can be written the following equalities:

$$\frac{dS_I}{dt} = -k_1 \cdot \mu_1 \cdot X_I(t) = -k_1 \cdot \frac{dX_I}{dt} \quad (10)$$

by integrating this differential equation, one gets the following linear relationship between  $S_I(t)$  and  $X_I(t)$  that is:

$$S_I(t) = -k_1 \cdot X_I(t) + S_{I0} + k_1 \cdot X_{I0} \quad (11)$$

where  $X_{I0}$  and  $S_{I0}$  are respectively the initial values of  $X_I(t)$  and  $S_I(t)$ .

To explicit  $X_I(t)$ , let's replace  $\mu_I$  in (10) by its expression in (1) so that one gets the following relationship:

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

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

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

with:  $a = S_{I0} + k_1 \cdot X_{I0}$

The expression (13) can be written in the following form by separating the variables from both sides:

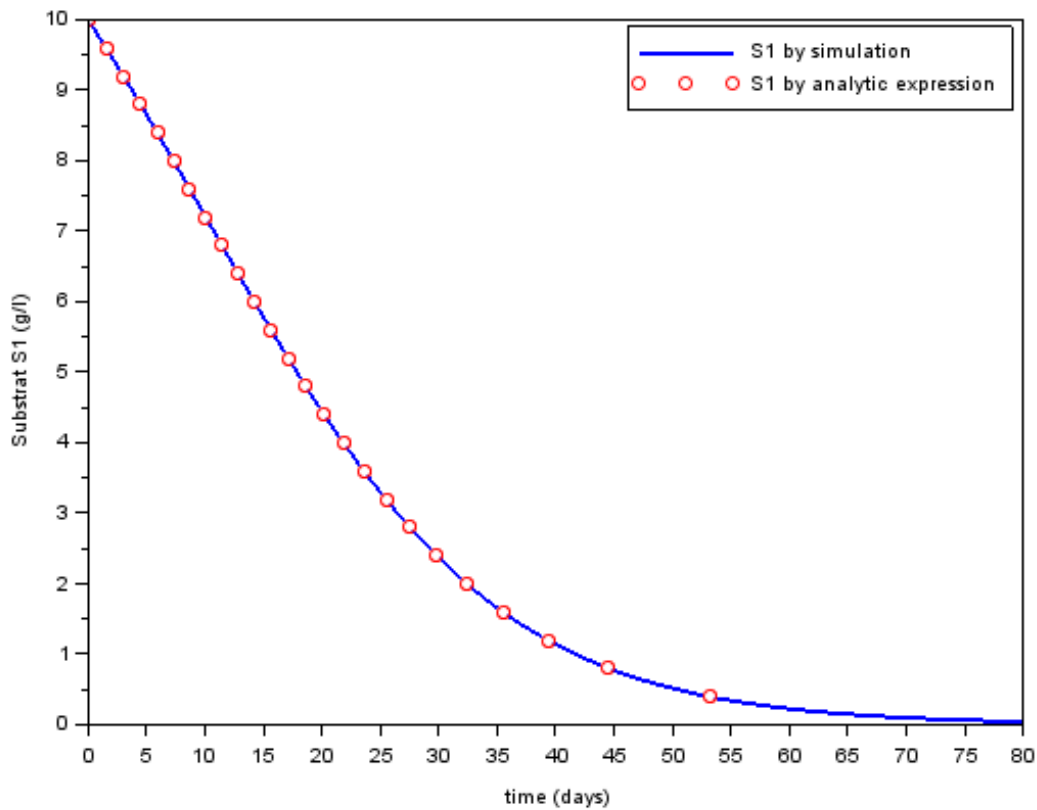
$$\frac{(S_1 + K_{S1})}{S_1 \cdot (S_1 - a)} \cdot \frac{dS_1}{dt} = \mu_{1m} \quad (14)$$

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

$$t = f(S_1) = \frac{(K_{S1} + a)}{a \cdot \mu_{1m}} \cdot \ln\left(\frac{|S_1 - a|}{|S_{I0} - a|}\right) - \frac{K_{S1}}{a \cdot \mu_{1m}} \cdot \ln\left(\frac{|S_1|}{|S_{I0}|}\right) \quad (15)$$

It is not possible to express explicitly  $S_I(t)$  in a standard form. However, from (15),  $S_I(t)$  can be easily computed and graphically represented as shown in *fig.1* by just giving values to  $S_I$  and computing the corresponding time  $t$ . Expression (15),  $t=f(S_I)$  or  $S_I(t) = f^{-1}(t)$  are the analytical functions that contain the model parameters ( $K_{S1}$ ,  $\mu_{1m}$ ,  $k_I$ ) and initial values ( $S_{I0}$ ,  $X_{I0}$ ). This enables to study analytically the interaction and the influence of any of the involved parameters ( $K_{S1}$ ,  $\mu_{1m}$ ,  $k_I$ ) or initial values ( $S_{I0}$ ,  $X_{I0}$ ) on the dynamical evolution of the process  $S_I(t)$  that is the concentration of the substrate of carbonaceous material. The profiles of  $S_I(t)$

obtained by the analytical function (15) and that obtained by solving the system of differential equations are presented on the same graphic as implemented under Scilab software. They appear superimposed in the graphics of *fig.1* and thus are similar.



*Fig. 1. Temporal Evolution of  $S_1(t)$  by simulation and analytically*

### 3.2. 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 written in a standard form but can be expressed in the inverse form:  $t = g(X_1)$ . Therefore, the analytical expression is the function  $t = g(X_1)$ :

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

The analytical expression (17) includes the model parameters ( $K_{S1}$ ,  $\mu_{1m}$ ,  $k_1$ ) and the initial values ( $S_{10}$ ,  $X_{10}$ ). It enables to analyze the evolution of the concentration of the acidogenic

bacteria population as well as its sensitivity to the related model parameters. By varying the values of  $X_I$ , the values of corresponding time are computed and the function  $X_I = g^I(t)$  can be drawn. Graphics of  $X_I(t)$  obtained by simulation and by the analytical expression (17) are presented in Fig. 2. They appear superimposed and thus are similar.

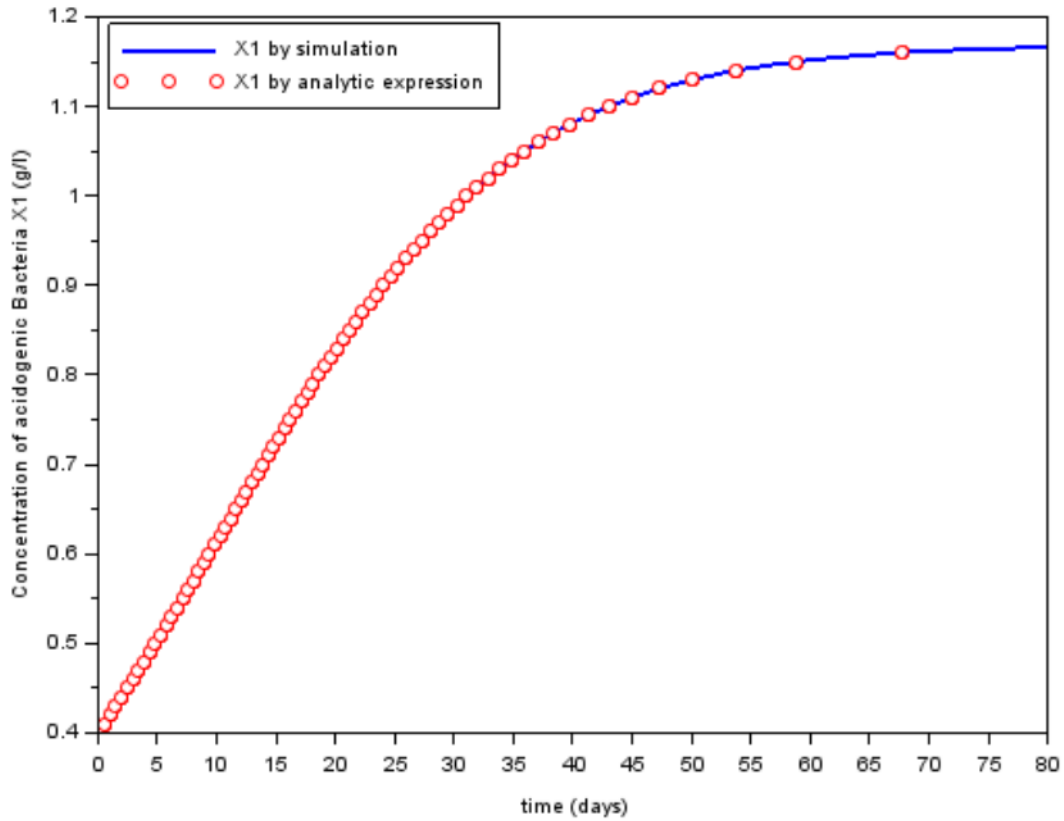


Fig.2. Temporal Evolution of  $X_I(t)$  by simulation and analytically

### 3.3. Some Remarks

#### 3.3.1. Behavior evolution of $S_I(t)$ and $X_I(t)$

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

$$\frac{dX_1}{dt} = \mu_{1m} \cdot \frac{S_1}{(S_1 + K_{S1})} \cdot X_1 = \mu_{1m} \cdot \frac{(-k_1 \cdot X_1 + a) \cdot X_1}{(-k_1 \cdot X_1 + K_{S1} + a)} = 0 \tag{18}$$

This leads to the condition:  $-k_1 \cdot X_1 + a = 0$ , which consequently leads to the asymptotic steady state value of acidogenic bacteria:  $X_I(t) = X_{1S} = \frac{a}{k_1} = X_{10} + \frac{S_{10}}{k_1} \cong 1.17 \text{ g/l}$ .

Similarly, from equation (11), we can determine the asymptotic steady state value for  $S_I(t)$  which is zero. This means that the concentration of the substrate of carbonaceous material will be almost completely consumed at relatively large time durations.

### 3.3.2. Settling time for $X_I(t)$ and $S_I(t)$

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  $X_I(t)$ , it corresponds to:  $X_I(t_{set}) = X_{Iset} = 0.95 \cdot X_{IS} = 1.11$  g/l. By replacing this settling value  $X_I$  set in (12), the settling time  $t_s$  is about 45 days. From equation (11), we can estimate the settling value for  $S_I(t)$  which is about 50 days. The comparison of these results is in full agreement with those given by simulation of the system of differential equations composing AM2 model.

### 3.3.3. Sensitivity analysis

Given the analytical relations (15) and (17), the analysis of the evolution of the substrate  $S_I(t)$  and of the bacteria  $X_I(t)$  with respect to all involved model parameters as well as their sensitivity can be easily performed analytically from these expressions.

## 4. TEMPORAL EVOLUTION OF $X_2(t)$ AND $S_2(t)$

### 4.1. Establishment of differential equations for $X_2(t)$ and $S_2(t)$

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

$$\frac{dX_2}{dt} = \mu_2 \cdot X_2 = \mu_{2m} \cdot \frac{S_2}{S_2 + \frac{S_2^2}{K_{I2}} + K_{S2}} \cdot X_2 \quad (19)$$

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

$$\frac{dS_2}{dt} = k_2 \frac{dX_1}{dt} - k_3 \cdot \frac{dX_2}{dt} \quad (20)$$

by integrating this last equation (20), we obtain:

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



which can also be written as:

$$S_2(t) = -k_3 X_2(t) + k_2 X_1(t) + C = -k_3 X_2(t) + f(t) \quad (22)$$

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

By replacing  $S_2(t)$  from (22) into the (19), we can explicit a non linear differential equation of the first order on  $X_2(t)$  which depends on  $X_1(t)$  via the term  $b(t)$ :

$$\frac{dX_2}{dt} = \mu_{2m} \cdot \frac{(-k_3 X_2 + f) X_2}{\left[ (-k_3 X_2 + f) + \frac{(-k_3 X_2 + f)^2}{K_{I2}} + K_{S2} \right]} = g(X_2, X_1) \quad (23)$$

Under this form, the differential equation (23) 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 given by (17). However, we can integrate (23) by numerical methods without the need to solve the system of coupled differential equations. But it requires to provide the values of  $X_1(t)$  at each step of integration by tabulation or by integrating the inverse of  $X_2(t)$  which is:

$$\frac{dt}{dX_2} = g^{-1}(X_2, X_1) \quad (24)$$

This differential equation contains all the model parameters ( $\mu_{2max}$ ,  $K_{S2}$ ,  $K_{I2}$ ,  $k_2$ ,  $k_3$ ) that affects the evolution of the methanogens as well as the corresponding initial conditions:  $S_{20}$ ,  $X_{20}$ . The other parameters concerning the acidogenic bacteria with their initial conditions are introduced in (23) by  $b(t)$  which is linked to  $X_1(t)$ . At this level, integrating only (23) instead of solving the set of differential equations of the AM2 model, makes it easier to study and analyze the influence of all parameters and initial conditions on  $X_2(t)$ . Another easiest way consists of integrating (23) by using a piecewise linear approximation of  $X_1(t)$  derived from (17). Further, we will integrate the differential equation (23) using this linear piecewise approximation of  $X_1(t)$ . The results will be compared to simulation and to those of our analytical approach.

#### 4.2. 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 (22) and (23). That is the only way to make them amenable to expressions that are analytically integrable. To this purpose, we consider a first approximation that concerns  $X_1(t)$ . One appropriate simple simplification is to

use a piecewise linear approximation by two segments. The first segment corresponds to a linear approximation derived from (17) during the transient response. The second one consists of approximating  $X_1(t)$  by a horizontal line corresponding to the asymptotic steady state response. The point of junction between the two segments corresponds to the settling time of  $X_1(t)$ .

However, even by using a linear approximation of  $X_1(t)$  during the transient response,  $X_2(t)$  remains still dependant from time, then (23) cannot be solved analytically. To be solvable analytically, it needs to be simplified to the level that the grown law of the process of the methanogenic bacterial population becomes linear of the form:

$$\mu_2 = \frac{\mu_{2m}}{K_{S2}} \cdot S_2 \quad (25)$$

By adopting these simplifications, (23) can be written as follows:

$$\frac{dX_2}{dt} = \mu_{2m} \cdot \frac{S_2}{K_{S2}} \cdot X_2 = \mu_{2m} \cdot \frac{(-k_3 \cdot X_2 + k_2 \cdot X_1 + C) \cdot X_2}{K_{S2}} = \mu_{2m} \cdot \frac{f(t) \cdot X_2 - k_3 \cdot X_2^2}{K_{S2}} \quad (26)$$

Now, the differential equation (26) corresponds to Bernoulli's equation [12] can be rewritten to match the standard form of Bernoulli's differential equation for the case where the coefficient  $n = 2$ ; that is:

$$\frac{dy(t)}{dt} + P(t) \cdot y(t) = Q(t) \cdot y^2(t) \quad (27)$$

Equation (246) structured in the standard Bernoulli's form becomes:

$$\frac{dX_2(t)}{dt} - \frac{\mu_{2m}}{K_{S2}} (C + k_2 \cdot X_1(t)) \cdot X_2(t) = -\frac{\mu_{2m}}{K_{S2}} \cdot k_3 \cdot X_2^2(t) \quad (28)$$

with

$$P(t) = -\frac{\mu_{2m}}{K_{S2}} (C + k_2 \cdot X_1(t)) \quad (29)$$

and

$$Q(t) = q_0 = -\frac{\mu_{2m}}{K_{S2}} \cdot k_3 \quad (30)$$

To solve (27), it is converted into another simpler differential equation of the first order that has a general solution [12]:

$$y(t) = \frac{\exp \int -P(t).dt}{C_0 - \int Q(t). \exp \int -P(t)dt} \tag{31}$$

To explicit the general solution in the form of (31), it requires the provision of  $P(t)$  which means in our case to provide the profile of  $X_I(t)$ . Here again, the problem of integrating this function is not obvious in standard analytical expressions. So, in this paper, we will use a piecewise linear approximation for  $X_I(t)$  as announced.

## 5. DETERMINATION OF $X_2(t)$

### 5.1. Determination of $X_2(t)$ with linear approximation of $X_I(t)$

The linear approximation of  $X_I(t)$  to the first order during the transient response is given from (17) by considering:

$$\ln(x) \cong x - 1 \tag{32}$$

By applying this approximation, relation (17) can be written in a linear form such as:

$$X_1(t) \cong X_{10} + u_0.t \tag{33}$$

with:

$$u_0 = \mu_{1m} \cdot \frac{(k_1 \cdot X_{10} - a) \cdot X_{10}}{(k_1 \cdot X_{10} - a - K_{s1})} = \mu_{1m} \cdot \frac{S_{10}}{(S_{10} + K_{s1})} \cdot X_{10} \tag{34}$$

It follows from (29) that  $P(t)$  is also linear with respect to time:

$$P(t) \cong -\frac{\mu_{2m}}{Ks2} (C + k_2 \cdot X_1(t)) = a_1 + b_1.t \tag{35}$$

with:

$$a_1 = -\frac{\mu_{2m}}{Ks2} \cdot (S_{20} + k_3 \cdot X_{20}) \tag{36}$$

$$b_1 \equiv -\frac{\mu_{2m} \cdot k_2}{Ks2} u_0 = -\frac{\mu_{2m} \cdot k_2}{Ks2} \cdot \mu_{1m} \cdot \frac{S_{10}}{(S_{10} + Ks1)} \cdot X_{10} \tag{37}$$

and

$$Q(t) = q_0 = -\frac{\mu_{2m}}{Ks2} \cdot k_3 \tag{38}$$

Having determined the expressions of  $P(t)$  and  $Q(t)$  according to the general solution (31), we can integrate the expressions in its numerator and in the denominator. The numerator in (31) equals:

$$N(t) = \exp\left(\int_0^t (-P_1(t)) \cdot dt\right) = \exp\left(-a_1 \cdot t - \frac{b_1}{2} \cdot t^2\right) \tag{39}$$

by introducing the initial value  $X_2(0)$  that is  $X_{20}$ , (31) becomes:

$$X_2(t) = \frac{X_{20} \cdot e^{-a_1 \cdot t - \frac{b_1}{2} \cdot t^2}}{1 - X_{20} \cdot q_0 \cdot \int_0^t e^{-a_1 \cdot t - \frac{b_1}{2} \cdot t^2} \cdot dt} \tag{40}$$

The integral in the denominator is a special mathematical function that depends on the values of the coefficients ( $a_1, b_1$ ). Its behaviour depends particularly on the sign of the term ( $-b_1$ ). In our case,  $b_1$  is negative, thus ( $-b_1$ ) is positif. Therefore, the corresponding integral leads to a function known as the imaginary error function  $erfi(x)$  which is defined as [13]:

$$erfi(t) = \frac{2}{\sqrt{\pi}} \cdot \int_0^t e^{z^2} \cdot dz \tag{41}$$

In case where the coefficients ( $\alpha, \beta$ ) are both positive, the integral in the denominator in expression (40) becomes according to [13]:

$$D(t) = \int_0^t e^{\alpha t + \beta t^2} dt = -\frac{\sqrt{\pi}}{2\sqrt{\beta}} \cdot \exp\left(-\frac{a^2}{4\beta}\right) \cdot \operatorname{erfi}\left(\frac{2\beta t + \alpha}{2\sqrt{\beta}}\right) \quad (42)$$

Since in our approximation,  $\alpha = -a_1$  and  $\beta = -b_1 / 2$  then, the final expression of  $X_2(t)$  under the set of adopted approximations is finally:

$$X_2(t) = \frac{X_{20} \cdot \exp\left(-a_1 t - \frac{b_1}{2} t^2\right)}{1 - X_{20} \cdot q_0 \cdot \frac{\sqrt{\pi}}{\sqrt{-2b_1}} \cdot \exp\left(\frac{a_1^2}{2b_1}\right) \cdot \operatorname{erfi}\left(\frac{-b_1 t - a_1}{\sqrt{-2b_1}}\right)} \quad (43)$$

This expression shows the temporal evolution of  $X_2(t)$  during the transient response of the processes. We can observe the presence of all the involved model parameters except  $K_{12}$  which has been neglected for the seek of approximations and simplifications. The presence of all the model parameters in expression (43) proves and explains the complex sensitivity and interactivity of biotechnological problems. This explains the sensitivity of the methane production as a final product with respect to all these parameters and conditions.

Expression (43) is mainly valid for the duration of the transient response. After that, it must be approximated by an asymptotic horizontal line corresponding to the steady state response. The steady state value of  $X_2(t)$  can be determined from the expression derived from (21):

$$X_2(t) = \frac{1}{k_3} (k_2 X_1(t) - S_2(t) + C) \quad (44)$$

For large values of the time,  $X_1(t)$  tends to  $(X_{1S} = a / k_1)$  and  $S_2(t)$  tends to zero; then the asymptotic value of  $X_{2S}$  corresponding to the steady state response is:

$$X_2(\infty) = X_{2S} = \frac{1}{k_3} \left( k_2 \cdot \frac{a}{k_1} + C \right) = \frac{1}{k_3} \left[ \frac{k_2}{k_1} \cdot S_{10} + S_{20} + k_3 \cdot X_{10} \right] \equiv 0.52 \text{ g/l} \quad (45)$$

*Fig. 3* represents the temporal evolution of  $X_2(t)$  obtained by simulation (blue curve); by the analytical expression (43) and (45) (black curve) and by integration of (23) using the piecewise linear approximation of  $X_1(t)$  (red curve) The analytical curves corresponding to expression (43) is limited by its asymptotic value at about  $t = 45 \text{ days}$  where  $X_2(t)$  reaches  $X_{2S}$ .

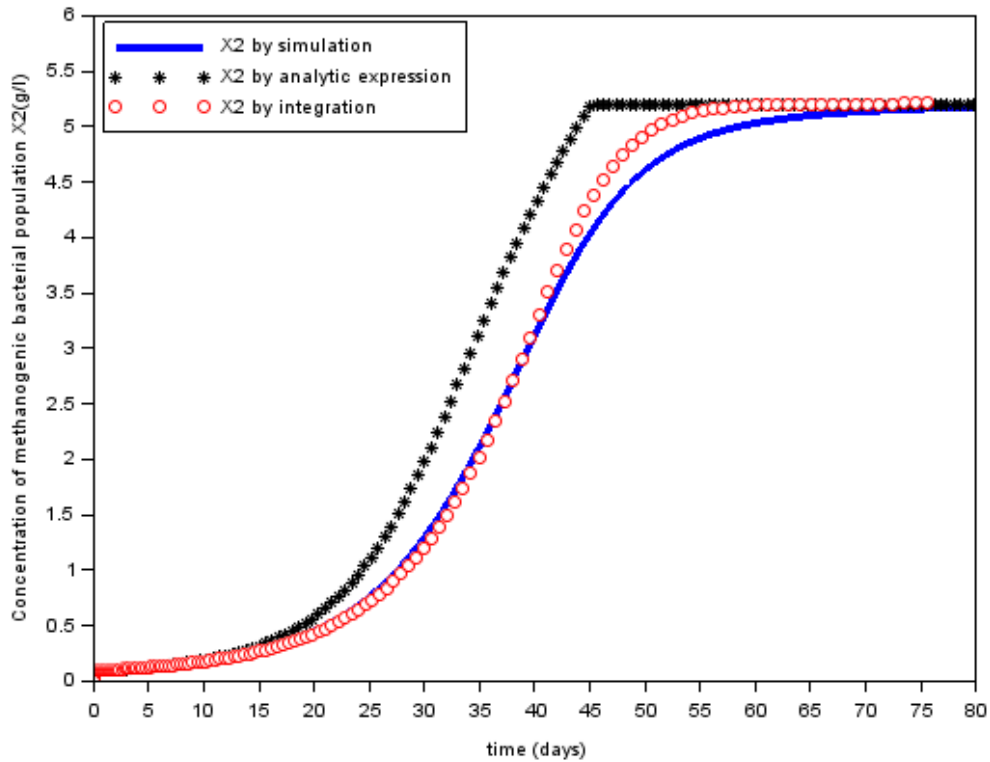


Fig. 3. Temporal evolution of  $X_2(t)$  by simulation and analytically

Although, the curve obtained by simulation is considered as the reference, the comparisons of the two other curves to that reference show some difference due to the adopted approximations. However, there is a quantitative agreement during the beginning of the process during about the 15 first days. Then, after that, there is a qualitative agreement. For long durations corresponding to the steady state response, the curves meet and are almost similar.

### 5.2. Evolution of substrate $S_2(t)$ under linear approximation of $X_1(t)$

By replacing  $X_2(t)$  and  $X_1(t)$  with their respective expressions in expression (21), we obtain the temporal evolution of the profile of the substrate  $S_2(t)$  in the analytical form.

$$S_2(t) = \frac{-k_3 \cdot X_{20} \cdot \exp(-a_1 t - \frac{b_1}{2} t^2)}{1 - X_{20} \cdot q_0 \cdot \frac{\sqrt{\pi}}{\sqrt{-2 \cdot b_1}} \cdot \exp(\frac{a_1^2}{2b_1}) \cdot \operatorname{erfi}(\frac{-b_1 t - a_1}{\sqrt{-2 \cdot b_1}})} + k_2 \cdot (X_{10} + u_0 t) + C \quad (46)$$

Fig. 4 represents the temporal evolution of  $S_2(t)$  obtained by simulation (blue curve); by the analytical expression (46) (black curve) and by numerical integration derived from (23) using the piecewise linear approximation of  $X_1(t)$  (red curve). The analytical expressions  $S_2(t)$  contains the parameters involved in the process and reveal their complex interaction with the

biological processes. This expression is an approximation during the beginning of the process that corresponds to the transient responses. At large time duration,  $S_2(t)$  vanishes after about 60 days.

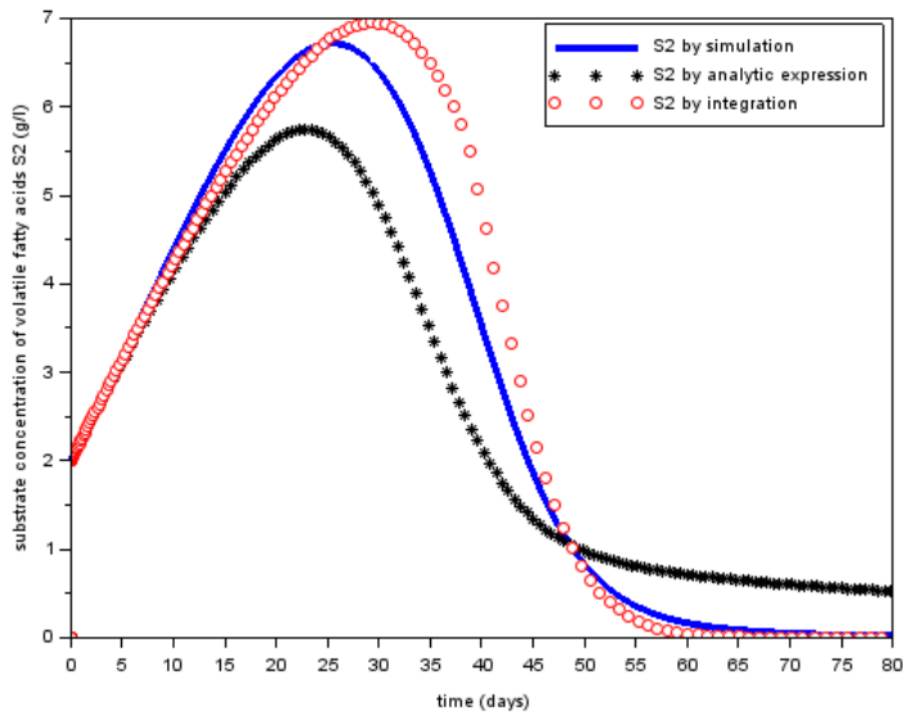


Fig. 4. Temporal evolution of  $S_2(t)$  by simulation and analytically

Comparing the other curves to the blue one that constitutes the reference, there curves are in quantitatively in agreement during the 20 first days at the beginning of generation of the processes. After that, there are differences because of the adopted approximations and because of the change on the slope of  $S_2(t)$  during the remaining period of the transient response. In this part, the linear approximations of  $X_1(t)$  and that of  $\mu_2$  in (23) can't hold anymore. Nevertheless, despite the used approximations used, there is a qualitative agreement that enables to analyze the influence of the parameters involved in the processes. Qualitatively, the profile of the analytical expression  $S_2(t)$  is roughly reproduced compared to that obtained one by solving the system of differential equations.

### 5.3. Evaluation of Methane Production

To estimate the methane production from the AM2 model, the literature provides data corresponding to a value of  $k_4$  which is closer to  $75 \text{ l}^2/\text{mg}$  [4]. According to this model, the temporal evolution of methane flow  $Q_{CH_4}(t)$  is computed from the expression (7) as follows:

$$Q_{CH_4}(t) = k_4 \cdot \mu_2 \cdot X_2(t) = k_4 \cdot \frac{dX_2}{dt} \quad (47)$$

The cumulated quantity of methane  $C_m(t)$  over a given period is obtained by integrating  $Q_{CH_4}(t)$  which is proportional to  $X_2(t)$ :

$$C_m(t) = \int k_4 \cdot \frac{dX_2}{dt} dt = k_4 \cdot X_2(t) \quad (48)$$

The production of the methane depends on the derivative of  $X_2(t)$  from the analytical expression (44), we can see the influence of almost all parameters involved in the AM2 model and then the sensitivity of the methane production to them. However, the cumulated quantity of methane depends only on  $X_2(t)$ . In case of batch reactors,  $X_2(t)$  tends after a transient period to a steady state response where  $X_2(t)$  becomes constant. It can be evaluated by the expression derived from (45):

$$C_m = k_4 \cdot X_2(\infty) = k_4 \cdot X_{2s} = \frac{k_4}{k_3} \left[ \frac{k_2}{k_1} \cdot S_{10} + S_{20} + k_3 \cdot X_{10} \right] \quad (49)$$

In this expression, one can notice that it does not contain the parameters of bacteria's growth rate which are mainly active during the transient period.

## 6. CONCLUSION

As an alternative to simulation by solving the system of differential equations characterizing the AM2 model, an analytical approach is proposed in case of batch reactors. It consists of adopting some approximations to reduce the mathematical complexity of the coupled differential equations. Analytical expressions for the state variables have been derived incorporating the model parameters and initial conditions revealing the complexity of the biotechnological systems. The proposed analytic expressions enable thus to perform a relatively easy analysis of the evolution of the main processes as well as the influence of the different parameters and initial conditions. The comparison of the results provided by this analytical approach to the numerical simulation shows a satisfying qualitative convergence of the former and therefore may justify its use under the adopted assumptions. It also opens some perspectives for improving and optimizing the biotechnological processes involved in such models.

**Conflict of Interest:** The author declares that he has no conflict of interest.



## REFERENCES

- [1] M. Gerber and R. Span, *An Analysis of Available Mathematical Models for Anaerobic Digestion of Organic Substances for Production of Biogas*, International Gas Union Research Conferences. IGRC, 2008.
- [2] I. Simonov, V. Lubenova, and I. Queinec, *Parameter and State Estimation of an Anaerobic Digestion of Organic Wastes Model with Addition of Stimulating Substances*, Bioautomation, Vol. 12, pp. 8-105, 2009.
- [3] H. Jagadish, et al., *Kinetics of Anaerobic Digestion of Water Hyacinth Using Poultry Litter as Inoculum*, International Journal of Environmental Science and Development, Vol. 3, No. 2, 2012.
- [4] A. Zaatri and R. Kelalaia, *Analysis and Simulation of AM2 Model for Anaerobic Digesters*, Banat's Journal of Biotechnology, Banat's Journal of Biotechnology, 2020.
- [5] R. Dewil et al., *Anaerobic digestion of biomass and waste: current trends in mathematical modeling*, Proceedings of the 18th World Congress of the International Federation of Automatic Control, Milano (Italy) August 28 - September 2, 2011.
- [6] D. Van et al., *A new kinetic model for biogas production from co-digestion by batch mode*, Global J. Environ. Sci. Manage., 4(3). pp. 251-262, 2018.
- [7] M. Sbarciog, M. Loccufier, and E. Noldus, *Determination of appropriate operating strategies for anaerobic digestion systems*, Biochemical Engineering Journal, 51, pp. 180–188, 2010.
- [8] A. Zaatri, N. Azzizi, and R. Kelaiaia, *Mathematical modeling and energy estimation of anaerobic bioreactors*, Third International Conference on Energy, Materials, Applied Energetics and Pollution ICEMAEP2016, October 30-31, Constantine, Algeria, 2016,
- [9] T. Salvatori, et al., *Evaluation of Polynomial Models to Predict Methane Production in Batch Mode Bioreactors*, European Control Conference (ECC), June 29-July 1, Aalborg, Denmark, 2016.
- [10] Y. Pererva, et al, *Existing Empirical Kinetic Models in Biochemical Methane Potential (BMP) Testing, Their Selection and Numerical Solution*, Water, 12(6), 1831. 2020.
- [11] S. Annigeri, *An Introduction to Scilab*, [https://www.cse.iitb.ac.in/~sohoni/TD604/sundry/Scilab\\_Tutorial.pdf](https://www.cse.iitb.ac.in/~sohoni/TD604/sundry/Scilab_Tutorial.pdf), 2009.
- [12] A. E. Parker, *Solving Linear First-Order Differential Equations Bernoulli's (Almost) Variation of Parameters Method*, Differential Equations. 3, 2020.
- [13] M. Geller and E.W. Ng, *A Table of Integrals of the Error Functions*, Journal of Research of the National Bureau of Standards, Section B Mathematical Sciences, 73B (1), 1969.