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RESEARCH ARTICLE

MATHEMATICAL MODELING, ANALYSIS, AND SIMULATION OF THE DYNAMICS OF ANAEROBIC DIGESTION OF BIOMASS WASTE IN DISCONTINUOUS OPERATION

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ABSTRACT

In this paper, a new model of the anaerobic digestion of biomass waste in discontinuous operation is developed. It takes into account all its stages and is analyzed, and validated with data from related literature. It aims at better predicting the production of biogas. The methodology formulation of the new model is based, on the one hand, on the principles of energy conversion processes, the application of physicochemical laws, and the conservation of matter, and on the other hand, on the characteristics of the existing models which allow an optimal conversion. As results and conclusion, we demonstrate, through mathematical analysis, some experimental observations, namely the existence, uniqueness, positivity, and boundedness of the solutions of the new model. The validation tests of the model show that the dynamics of its solutions are in agreement with the experimental data of the literature. Stability in the production of biogas is observed from the 35th day. The results of these tests also make it possible to have and understand the evolution of variables that are not taken into account in the literature.

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INTRODUCTION

Also called methanation, anaerobic digestion is a natural process of transformation of organic matter through distinct microorganisms in the absence of oxygen (Maytre, 1994). It generally comprises four phases: hydrolysis, acidogenesis, acetogenesis, and methanogenesis, and therefore makes it possible to reduce the quantity of biomass waste and produce energy. It is influenced by several factors such as PH, temperature, the humidity of biomass waste, and physicochemical characteristics (Rouez, 2008). Different configurations of digesters can be adopted in anaerobic digestion. Depending on the origin of the material and according to the desired result at the end of the digestion, the biomass can be digested continuously, discontinuously (batch) or semi-continuously (fed-batch) in low or high temperatures, in one, two, three, or four stages (Arras). In the continuous mode of anaerobic digestion, the digester is fed with a constant flow, and the digestate is evacuated by mechanical action. This technology is ideal for large installations. The digesters used can be arranged both vertically and horizontally (PhD thesis, École de technologie supérieure, 2007). In semi-continuous mode, the digester is gradually filled according to the progress of the reactions to avoid overloading and promote growth. In the discontinuous operation of anaerobic digestion, the substrate is initially placed in the digester and the latter is hermetically sealed during the entire transformation period. When the quantity of biogas drops or when there is no longer any production of biogas, the digester is empty and we start the process again (Hess, 2007). This is how anaerobic digestion is mainly carried out today in most developing countries. At the end of the anaerobic digestion processes, it often happens that the quantity of biogas produced is very low or that the power methanogenic of biogas is very low, thus involving unnecessary expenses.

How to predict the quantity of biogas in advance?

How to control anaerobic digestion to optimize this quantity of biogas produced?

What are the parameters that act on the methanogenic power and on the production of biogas?

These questions raise the need for an analytical study to help engineering to optimize the process of anaerobic digestion of biomass waste. To control and optimize anaerobic digestion in order to provide approaches to answering these questions, mathematical models have been developed.

Thus, some models take into account one or two stages (Donoso-Bravo, 2011; PhD thesis, E'cole de technologie sup'erieure, 2007; Bernard, 2001; Arras; Rinco, 2014; Ouchtout, 2021), others three, four, or five stages depending on the case (Laraj, 2022; Fekih-Salem, 2011; J'ero'me, 2014; Daoud, 2017). The majority of these models are developed when the digester is operating continuously. Few works are available in the literature relating to the mathematical modeling of anaerobic digestion in discontinuous operation for its analysis, its control, its optimization and to better predict the production of biogas. Mathematical models of anaerobic digestion in discontinuous operation, at one stage (acidogenesis), and at two stages (hydrolysis and methanogenesis), have been respectively developed by Arras wassila (Arras) and Salih (Rincon, 2014). Recently, a mathematical model of anaerobic digestion in discontinuous operation with recirculation of leachates was proposed by Laraj (9). We propose to develop, analyze mathematically and simulate a mathematical model of anaerobic digestion with four stages (hydrolysis, acidogenesis, acetogenesis, and methanogenesis) by the discontinuous operation to help engineering and better predict biogas production during energy conversions.

Model development

Model assumption

- Anaerobic digestion is described by a four-step process (hydrolysis, acidogenesis, acetogenesis, and methanogenesis).
- The population of bacteria is divided into three groups of bacteria with homogeneous characteristics.
- The amount of carbon dioxide produced during hydrolysis is assumed to be negligible.
- Growth rates follow Monod kinetics (Harmand, 1942).
- Inhibition is not taken into account.
- All the quantity of dead bacteria constitutes a new substrate for the hydrolysis step.

Formulation and description of the model: The substrate compartment is divided into two parts: The slowly biodegradable substrate of concentration S_0 and the easily biodegradable substrate of concentration S_1 (Fekih-Salem, 2011). Thus, while the acidogenic bacteria degrade the substrate of concentration S_1 , the slowly biodegradable substrate is slowly transformed into an easily biodegradable substrate with the rate r_0 . r_0 can be $k_0 S_0$ or $k_0 S_1$ according to the two visions in practice in the literature. r_0 is a constant when hydrolysis is considered a purely enzymatic phenomenon without a hydrolytic microbial compartment. When considered as an enzymatic reaction with a hydrolytic microbial compartment, r_0 designates the specific growth rate of acidogenic bacteria of concentration X_0 on the slowly biodegradable substrate of concentration S_0 . In order not to drag a lot of symbols, we agree to designate a component and its concentration by the same letter. The hydrolysis reaction is as follows:



k_0 is the efficiency coefficient associated with the reaction.

By definition, the rate of a reaction is equal to the opposite of the rate at which one unit of the reactant disappears. It is also equal to the speed of creation of a unit of the product (15). Thus, from reaction (1) we have:

$$-\frac{dX_0}{dt} = \frac{1}{k_0} \frac{dS_1}{dt} = r_0 \quad (2)$$

As described and explained in (6), the acidogenesis reaction is as follows:



So,

$$-\frac{1}{k_1} \frac{dS_1}{dt} = \frac{X_1}{dt} = \frac{1}{k_2} \frac{dS_v}{dt} = \frac{1}{k_3} \frac{dCO_2}{dt} = \mu_1(S_1)X_1 \quad (4)$$

The substrate is composed of acetic acid, volatile fatty acid, alcohol, and hydrogen. Then, the substrate is consumed by acetogenic bacteria for their growth, and they are converted into carbon dioxide and substrate composed of acetic acid and hydrogen (13). The reaction of acetogenesis can be written as follows:



So,

$$-\frac{1}{k_4} \frac{dS_v}{dt} = \frac{X_v}{dt} = \frac{1}{k_5} \frac{dS_2}{dt} = \frac{1}{k_6} \frac{dCO_2}{dt} = \mu_v(S_v)X_v \quad (6)$$

In the final phase, the methanogenic bacteria of concentration X_2 consume the substrate and they are converted into carbon dioxide and methane. The methanogenesis reaction is as follows (6):



So,

$$-\frac{1}{k_7} \frac{dS_2}{dt} = \frac{X_2}{dt} = \frac{1}{k_9} \frac{dCH_4}{dt} = \frac{1}{k_8} \frac{dCO_2}{dt} = \mu_2(S_2)X_2 \tag{8}$$

$k_i; i = 0;1;2;3;4;5;6;7;8;9$ designate the efficiency coefficients associated with the reactions. $\mu_i(S_i); i=1;2$ the respective growth rates and are a function of the substrate. Growth rates are assumed to follow Monod kinetics (14). We therefore have:

$$\mu_i(S_i) = \frac{\mu_{m_i} S_i}{K_{S_i} + S_i} \text{ pour tout } i \in \{1;2\} \tag{9}$$

By the principle of conservation of mass, we have:

$$k_2 = f_2(k_1 - 1) \tag{10}$$

$$k_3 = (1 - f_2)(k_1 - 1) \tag{11}$$

$$k_5 = f_3(k_4 - 1) \tag{12}$$

$$k_6 = (1 - f_3)(k_4 - 1) \tag{13}$$

$$k_8 = (1 - f_4)(k_7 - 1) \tag{14}$$

$$k_9 = f_4(k_7 - 1) \tag{15}$$

Where α are the transformed proportions (See figure (1) and the system (Witelski, 2015) for more detail). In the continuous operation of anaerobic digestion, it is the rule rather than the exception not to take into account the mortality of bacteria. But in discontinuous operation, mortality cannot be neglected (Witelski, 2015). Also, dead bacteria constitute a new substrate for the hydrolysis stage (2,8). By denoting k_d as the mortality rate of bacteria, from (2),(4),(6), (8) and (9) the schematic view of the process (Figure 1) and the model that we propose are expressed as follows:

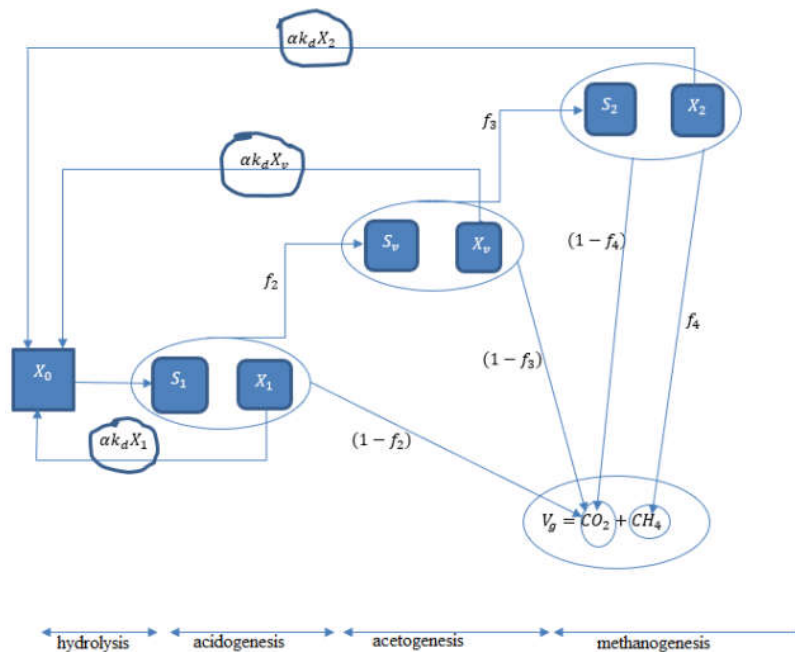


Figure 1: Schematic view used for modeling the process of anaerobic digestion. The parameter f_2 represents the part (proportion) of $(k_1 - 1) \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1$ transformed into S_v and $(1 - f_2)$ represents the part (proportion) transformed into CO_2 during the acidogenesis phase. The parameter f_3 represents the part (proportion) of $(k_4 - 1) \frac{\mu_{m_4}}{K_{S_v} + S_v} S_v X_v$ transformed into S_2 and $(1 - f_3)$ represents the part (proportion) transformed into CO_2 during the phase of acetogenesis. The parameter f_4 represents the part (proportion) of $(k_7 - 1) \frac{\mu_{m_7}}{K_{S_2} + S_2} S_2 X_2$ transformed into CH_4 and $(1 - f_4)$ represents the part (proportion) transformed into CO_2 during the phase of methanogenesis. α is the proportion of dead

bacteria transformed into the substrate for the hydrolysis step and we take in our work $\alpha = 1$.

$$\begin{cases} \frac{dX_0}{dt} = -k_h X_0 + \alpha k_d (X_1 + X_v + X_2) \\ \frac{dS_1}{dt} = k_0 k_h X_0 - k_1 \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 \\ \frac{dX_1}{dt} = \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 - k_d X_1 \\ \frac{dS_v}{dt} = k_2 \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 - k_4 \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v \\ \frac{dX_v}{dt} = \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v - k_d X_v \\ \frac{dS_2}{dt} = k_5 \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v - k_7 \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 \\ \frac{dX_2}{dt} = \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 - k_d X_2 \\ \frac{dV_g}{dt} = k_3 \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 + k_6 \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v + k_8 \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 + k_9 \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 \end{cases} \tag{16}$$

With the initial conditions

$$X_0(t_0) = X_{0_0}; S_1(t_0) = S_{1_0}; X_1(t_0) = X_{1_0}; S_v(t_0) = S_{v_0}; X_v(t_0) = X_{v_0}; S_2(t_0) = S_{2_0}; X_2(t_0) = X_{2_0}; V_g(t_0) = V_{g_0} \tag{17}$$

a is the proportion of dead bacteria transformed into the substrate for the hydrolysis step and we take in our work $a = 1$. V_g is the quantity of biogas ($CO_2 + CH_4$) produced per unit volume at time t .

Hypotheses

Hypothesis 1 The coefficients $K_d, k_i; i = \{1;4;7\}, f_2, f_3$ and f_4 satisfy the following conditions:

$$0 < k_d < \min\{\mu_{m_1}; \mu_{m_v}; \mu_{m_2}\} \tag{18}$$

$$\forall i \in \{1;4;7\}; k_i > 1 \tag{19}$$

$$\forall i \in \{2;3;4\}; 0 < f_i < 1 \tag{20}$$

Hypothesis 2 The parameters $k_i; i = \{0;1;2;3;4;5;6;7;8;9\}$ are strictly positive and satisfy the following condition:

$$\frac{k_0}{k_1 k_4 k_7} (\alpha k_4 k_7 + \alpha k_2 k_7 + \alpha k_2 k_5 + k_3 k_4 k_7 + k_2 k_5 k_8 + k_2 k_5 k_9 + k_2 k_6 k_7) < 1, \tag{21}$$

MATHEMATICAL RESULTS

Existence and uniqueness of solutions

A solution of system (16) is a function

$$X : t \in [0; +\infty[\subset \mathbb{R} \rightarrow X(t) = (X_0(t); S_1(t); X_1(t); S_v(t); X_v(t); S_2(t); X_2(t); V_g(t))^T \in \mathbb{R}^8$$

Let $F : X \in \mathbb{R}^8 \rightarrow F(X) \in \mathbb{R}^8$ with

$$F(X) = \begin{cases} -k_h X_0 + \alpha k_d (X_1 + X_v + X_2) \\ k_0 k_h X_0 - k_1 \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 \\ \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 - k_d X_1 \\ k_2 \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 - k_4 \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v \\ \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v - k_d X_v \\ k_5 \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v - k_7 \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 \\ \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 - k_d X_2 \\ k_3 \frac{\mu_{m_1}}{K_{S_1} + S_1} S_1 X_1 + k_6 \frac{\mu_{m_v}}{K_{S_v} + S_v} S_v X_v + k_8 \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 + k_9 \frac{\mu_{m_2}}{K_{S_2} + S_2} S_2 X_2 \end{cases} \tag{22}$$

The system (16) becomes

$$\frac{dX}{dt} = F(X); \quad X(t_0) = (X_{0_0}; S_{1_0}; X_{1_0}; S_{v_0}; X_{v_0}; S_{2_0}; X_{2_0}; V_{g_0})^T \tag{23}$$

All partial derivatives of order 1 of F exist and are continuous at any point of its domain. F is therefore of class C^1 . Consequently, the initial value problem (23) admits a unique solution satisfying the fixed condition $X(t_0) = X_{00}; S_{10}; X_{10}; S_{v0}; X_{v0}; S_{20}; X_{20}; V_{g0} T$.

Positivity and boundedness of solutions

Lemme 3.2.1: Positivity of solutions

If $X_{00}; S_{10}; X_{10}; S_{v0}; X_{v0}; S_{20}; X_{20}$ et V_{g0} are all positive, then $X_0(t); S_1(t); X_1(t); S_v(t); X_v(t); S_2(t); X_2(t)$ and $V_g(t)$ remain positive for all $t \geq t_0$

Proof

Assume that $X_{00}; S_{10}; X_{10}; S_{v0}; X_{v0}; S_{20}; X_{20}$ et V_{g0} are all positive.

$\forall i \in \{1; v; 2\}$, $\frac{dX_i(t)}{dt} = (\frac{\mu_{m_i}}{K_{S_i} + S_i(t)} S_i(t) - k_d) X_i(t)$, then $X_i(t) = X_i(t_0) \exp(\int_{t_0}^t (\frac{\mu_{m_i}}{K_{S_i} + S_i(\tau)} S_i(\tau) - k_d) d\tau)$. Since $X_i(t_0) = X_{i0} \geq 0$, we have:

$$X_i(t) \geq 0, \forall i \in \{1; v; 2\} \text{ and } \forall t \geq t_0$$

By considering the first equation of the system (16) we have:

$$\begin{aligned} \frac{dX_0(t)}{dt} &= -k_h X_0(t) + k_d (X_1(t) + X_v(t) + X_2(t)) \\ &\geq -k_h X_0(t) \end{aligned}$$

By bringing the second member into the first and by multiplying the inequality by its integration factor, we obtain:

$e^{\int_{t_0}^t k_h ds} \frac{dX_0(t)}{dt} + k_h e^{\int_{t_0}^t k_h ds} X_0(t) \geq 0 \iff \frac{d}{dt} (e^{\int_{t_0}^t k_h ds} X_0(t)) \geq 0$. Then the function $t \mapsto e^{\int_{t_0}^t k_h ds} X_0(t)$ is increasing on $[t_0, +\infty[$. Therefore, $e^{\int_{t_0}^t k_h ds} X_0(t) \geq X_0(t_0)$ for all $t \in [t_0, +\infty[$. Thus, $X_0(t) \geq X_0(t_0) e^{-\int_{t_0}^t k_h ds}$. Since $X_0(t_0) \geq 0$, we conclude that $X_0(t) \geq 0$ for all $t \in [t_0, +\infty[$.

By considering the second equation of the system (16) we obtain:

$$\begin{aligned} \frac{dS_1(t)}{dt} &= k_0 k_h X_0(t) - k_1 \mu_1 (S_1(t)) X_1(t) \\ &\geq -k_1 \mu_1 (S_1(t)) X_1(t) \\ &\geq \frac{-k_1 \mu_{m_1} X_1(t)}{K_{S_1} + S_1(t)} S_1(t) \\ &\geq \alpha(t) S_1(t) \text{ avec } \alpha(t) = \frac{-k_1 \mu_{m_1} X_1(t)}{K_{S_1} + S_1(t)} \end{aligned}$$

By bringing the second member into the first and by multiplying the inequality by its integration factor, we obtain:

$S_1(t) \geq S_1(t_0) e^{\int_{t_0}^t \alpha(s) ds}$ for all $t \in [t_0, +\infty[$. Since $S_1(t_0) \geq 0$ and the exponential function is always positive and not zero, it is clear that $S_1(t) \geq 0$ for all $t \in [t_0, +\infty[$.

Using similar reasoning, we show that: $\forall t \in [t_0, +\infty[, X_1(t) \geq 0, S_v(t) \geq 0, X_v(t) \geq 0, S_2(t) \geq 0, X_2(t) \geq 0$ et $V_g(t) \geq 0$

Lemme 3.2.2: Boundedness of the solutions

Under **Hypothesis 1** and **Hypothesis 2**, the solutions of the system (16) remain bounded for all initial conditions of positive components

Proof

Let V be the function defined on $(t_0; +\infty[$ by

$$\begin{aligned} V(t) = X_0(t) + \alpha X_1(t) + \alpha X_v(t) + \alpha X_2(t) + \left(\frac{\alpha}{k_1} + \frac{\alpha k_2}{k_1 k_4} + \frac{\alpha k_2 k_5}{k_1 k_4 k_7} + \frac{k_3}{k_1} + \frac{(k_8 + k_9) k_2 k_5}{k_1 k_4 k_7} + \frac{k_2 k_6}{k_1 k_4} \right) S_1(t) \\ + \left(\frac{\alpha}{k_4} + \frac{\alpha k_5}{k_4 k_7} + \frac{(k_8 + k_9) k_5}{k_4 k_7} + \frac{k_6}{k_4} \right) S_v(t) + \left(\frac{\alpha}{k_7} + \frac{k_8 + k_9}{k_7} \right) S_2(t) + V_g(t) \end{aligned} \tag{24}$$

From the equations of the system (16), we have:

$$\frac{dV(t)}{dt} = k_h \left[\frac{k_0}{k_1 k_4 k_7} (\alpha k_4 k_7 + \alpha k_2 k_7 + \alpha k_2 k_5 + k_3 k_4 k_7 + k_2 k_5 k_8 + k_2 k_5 k_9 + k_2 k_6 k_7) - 1 \right] X_0(t) \tag{25}$$

Since $\frac{k_0}{k_1 k_4 k_7} (\alpha k_4 k_7 + \alpha k_2 k_7 + \alpha k_2 k_5 + k_3 k_4 k_7 + k_2 k_5 k_8 + k_2 k_5 k_9 + k_2 k_6 k_7) < 1$ and $X_0(t)$ remains positive. So the function V is decreasing.

Since V is lower bounded by zero, then $0 < \lim_{t \rightarrow +\infty} V(t) < \infty$.

Therefore, $X_0(t); S_1(t); X_1(t); S_v(t); X_v(t); S_2(t); X_2(t)$ and $V_g(t)$ are bounded on $[t_0; +\infty[$ (Since they are positive)

Validation tests of the new model (Numerical simulations)

To test our model, we compared the dynamics of the solutions of our model with the dynamics of the solutions of the Rouez's model (2). Thus, first, we reported the results of the simulations of the Rouez's model, and second, we presented the results of the simulations of our model for the different types of biomass used by Rouez. The biomasses used by Rouez are household and similar waste (leftovers from meals, expired products, food plastics, etc.). These biomasses are categorized and are denoted FG, MAT, BOIS, etc. according to their components. Our simulation results are obtained using the ode45 function of MATLAB. The majority of the values of the parameters of our model are taken from (2). The values of the other (new) parameters are assumed. The simulation results are as follows.

For biomass waste noted FG

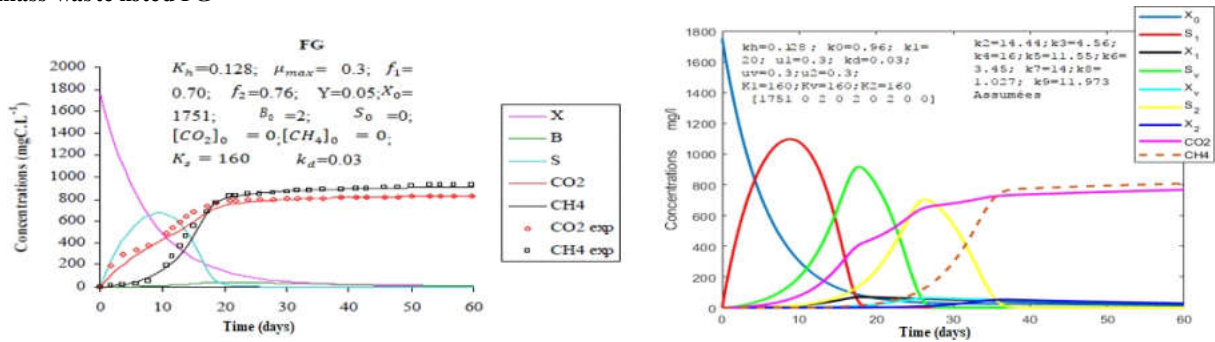


Figure 2. Left. The dynamics of the solutions of the Rouez model and the dynamics of the experimental data for the noted biomass FG (2). Right: The dynamics of the solutions of the model (16).

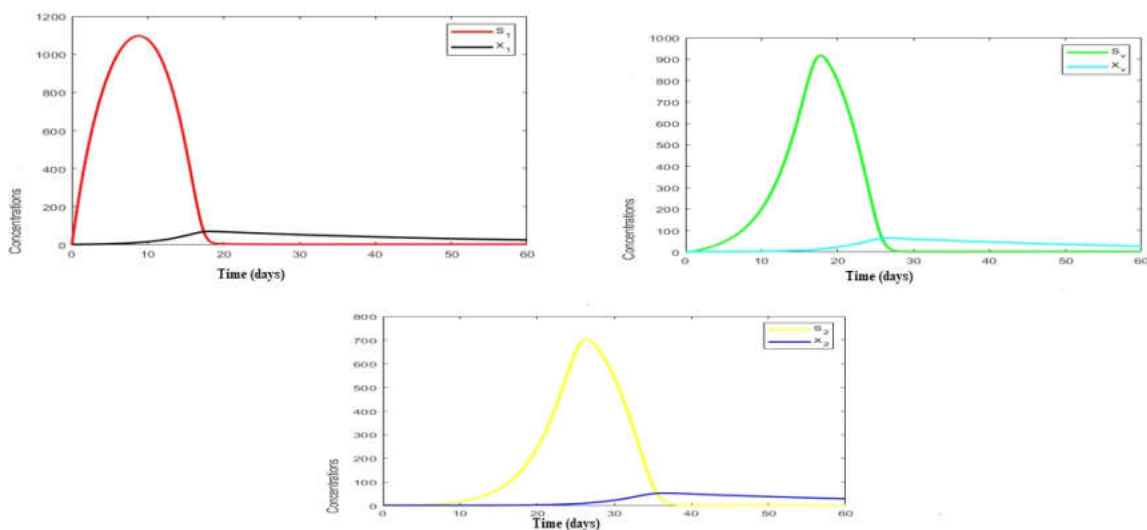


Figure 3. The dynamics of $S_1; X_1; S_v; X_v; S_2; X_2$ for the model (16) with the biomass noted FG

For biomass waste noted MAT

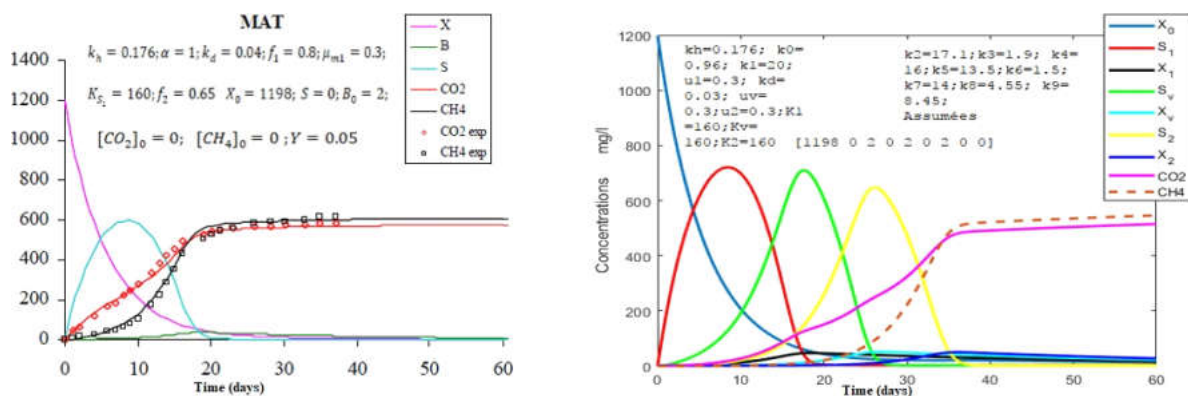


Figure 4. Left:: The dynamics of the solutions of the Rouez model and the dynamics of the experimental data for the noted biomass MAT(2). Right:: The dynamics of the solutions of the model (16).

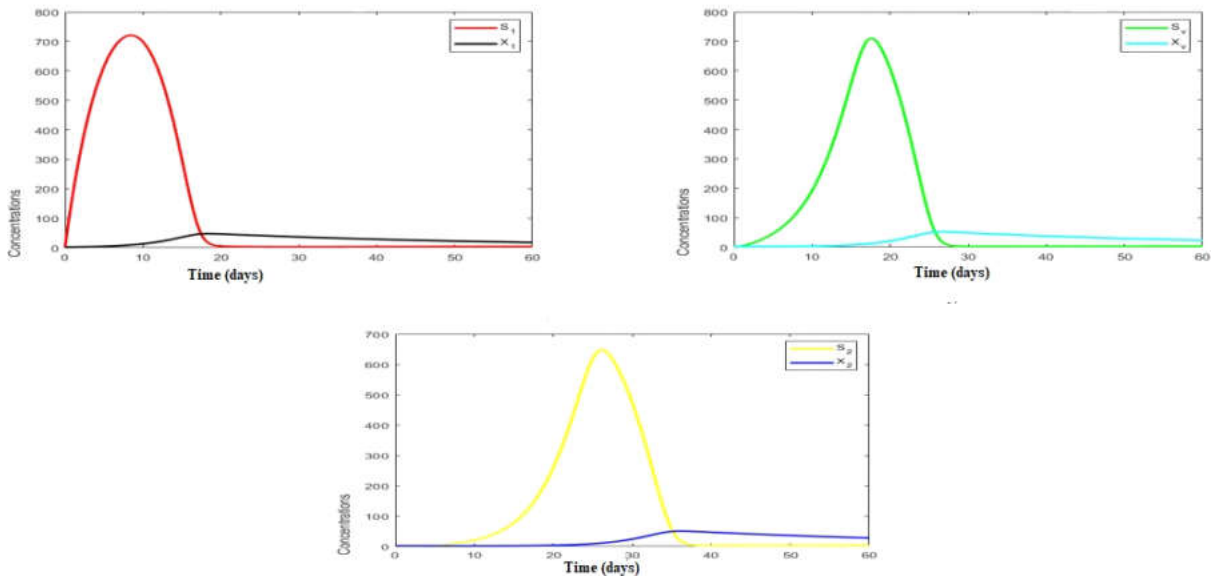


Figure 5. The dynamics of $S_1; X_1; S_v; X_v; S_2; X_2$ for the model (16) with the biomass noted MAT

For biomass waste noted BOIS

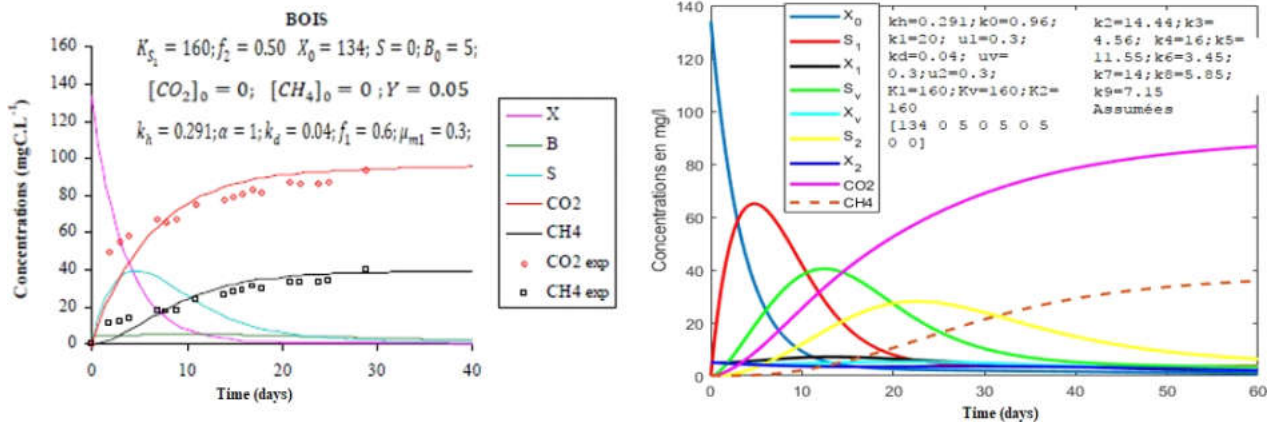


Figure 6. Left. The dynamics of the solutions of the Rouez model and the dynamics of the experimental data for the noted biomass BOIS(2). Right:: The dynamics of the solutions of the model (16)

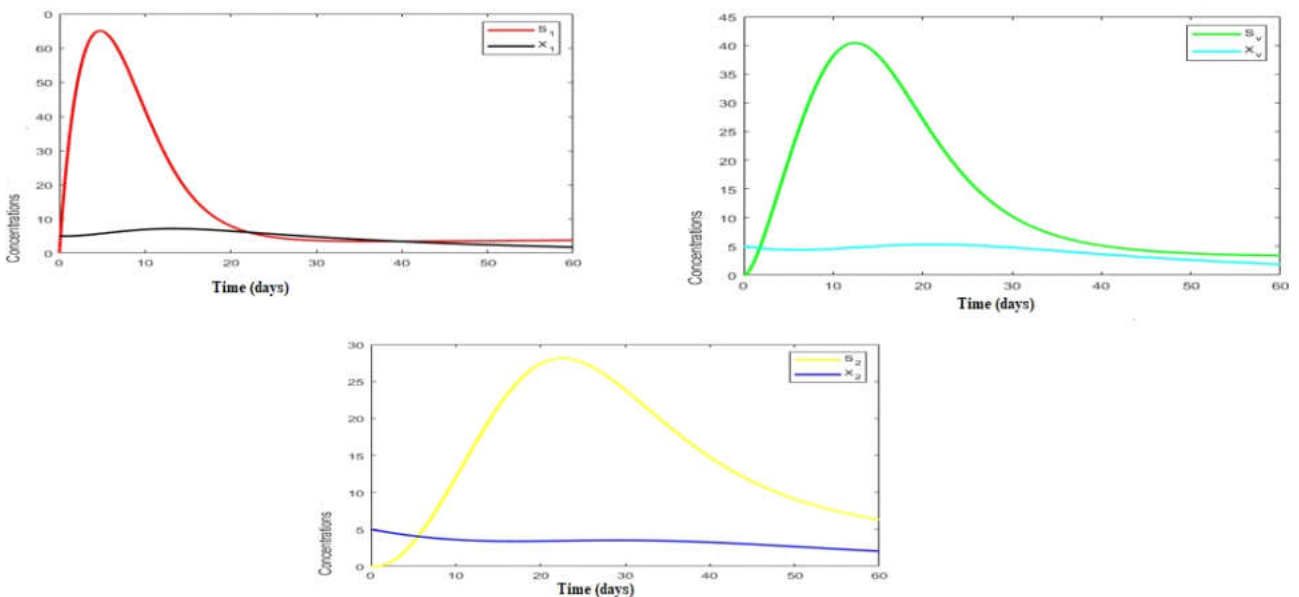


Figure 7. The dynamics of $S_1; X_1; S_v; X_v; S_2; X_2$ for the model (16) with the biomass noted BOIS

The comparison of the evolution of the solutions of our model and that of Rouez shows that our model is in agreement with the data experimental data obtained by Rouez. There is a correlation between the dynamics of the solutions of our model and the experimental data of Rouez. Our model thus makes it possible to predict the production of biogas. Stability in the production of biogas is observed from the 35 days (See Figures 2;4 and 6). Our model also makes it possible to have and understand the dynamics of the variables which are not taken into account by Rouez (2), in particular the concentration of acidogenic bacteria, the concentration of acetogenic bacteria, the concentration of easily biodegradable substrate, and the concentration of acid (See Figures 3; 5 and 7).

CONCLUSION

A mathematical model involved in the energy conversion of biomass waste in discontinuous operation has been developed and analyzed to help the engineer to predict the performance of the reactors without necessarily taking the phase of realization and experimentation. We are interested in the process of anaerobic digestion for the production of biogas in a digester in discontinuous operation. Modeling this mode of conversion is an essential tool for predicting biogas production. The new model of ordinary differential equations takes into account all stages of anaerobic digestion in batch operation. This model, which was not available in the literature, was analyzed mathematically. The existence, uniqueness, positivity, and boundedness of the solutions of the model are proven. The validation tests of the model have shown that the dynamics of its solutions are in agreement with the experimental data of the literature. The results of these tests made it possible to have and understand the evolution of the variables which are not taken into account in the literature.

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