An Efficient Visible Numerical Model to Find the Optimal Anaerobic Digestion Temperature in a Continuous Reactor Without Hydrolytic Microbial Compartment

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Abstract

Although the methanization process is already a relatively advanced and widely used technology, its control on an industrial scale is still the subject of extensive research. The search for appropriate models to be used in control theory is now a high priority to optimize fermentation processes and solve important problems related to process instability. The aim of this study is to prove how it is possible to find the digestion temperature for which biogas production is optimal, without going through an experiment. For this purpose, we have developed a numerical model based on mass balances, performed on microorganisms and organic substrates. This model predicts the cumulative volume, volume flow rate, and molar composition of biogas (methane and carbon dioxide) as a function of temperature. The influence of temperature on digestion was studied in the range of 20 to 40 °C in mesophilic regime. The results show that the daily production, the cumulative volume, and the molar composition of the biogas are more influenced by the temperature inside the reactor. The cumulative volume of biogas increases as the temperature increases in the range of 20 °C-35 °C and peaks at 35 °C.

Keywords: Methanization; Biogas; Modeling; Temperature; Methane.

Received: 12 May 2021; Revised: 26 July 2021; Accepted: 03 August 2021.

Article type: Research article.

1. Introduction

The current global energy system is characterized by a dependence on fossil fuels. The consumption of fossil resources, whether for the production of goods or energy, causes an increase in greenhouse gases which are the main cause of global warming.^[1]

Nowadays, the development of new energy sources has become a priority in the fight against climate change. Renewable energies from biomass, especially biogas from the methanization of organic matter, are attracting increasing interest. Anaerobic digestion is a natural process of decomposition of organic matter by bacteria in anaerobic conditions. This decomposition leads to the formation of biogas rich in methane (CH₄), thus forming a renewable energy source.

The anaerobic digestion process still faces many challenges, although this process is already a relatively

advanced and widely used technology to treat sewage sludge and wastewater.^[2,3] However, due to the complexity of biochemical mechanisms and the specific experimental conditions of each bioreactor, there are some technical problems related to the instability of the process, the optimization of the production and the optimal operating conditions of the process.

The modeling of the methanization process is then presented as a suitable solution able to overcome the problems of optimization of the biogas production.

Several mathematical models of bioreactors have been proposed. The main models cited in the literature in terms of anaerobic digestion are phenomenological and empirical, models dedicated to the control and observation of anaerobic digestion systems.^[4-6]

The present work fills a scientific gap in terms of models for predicting total biogas production as a function of digestion temperature. This model will take into account a minimal level of complexity required to represent the biogas productions obtained during different anaerobic incubations. It aims to prove how it is possible to increase the quantity and quality of biogas by acting on the temperature within the digesters, without having to go through an experiment.

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The main objective of the present work is to develop a numerical model able to provide the optimal temperature for anaerobic digestion. The originality of this model lies in its simpler way of modeling the dynamics of carbon dioxide in the liquid phase, contrary to several models using acid-base reactions.

The interest of this work is to apprehend more knowledge in the field of biogas production in order to contribute in an innovative way to the development of this very promising field.

1.1 Mechanism of anaerobic digestion

Biogas production proceeds in a succession of four distinct stages (Fig. 1), each with its characteristic microbial population. The output produced by each population becomes the input for the next population. The four main steps are presented below:

Fig. 1 Metabolic fluxes of anaerobic digestion.

Hydrolysis: the first step by which macromolecules break down in the presence of water, into small soluble molecules at the origin of the fermentation juice.

Acidogenesis: second stage during which the simple molecules are transformed, under the effect of bacteria in acids of low molecular weight (lactic acid or volatile fatty acids) and alcohols such as ethanol, bicarbonate, and molecular hydrogen.

Acetogenesis: a stage in which acetogenic and sulfate-reducing bacteria transform some of the products of the previous stages so that they can effectively produce methane.

Methanogenesis: the last phase during which acetate is reduced to methane and bicarbonate which in turn is reduced by hydrogenating bacteria to methane.

1.2. Phase transfer in an anaerobic digestion medium

In the processes of putting in contact a liquid phase with a gas phase, phenomena of transfer of matter between these two phases exist. These phenomena are described by Henry's law, according to which the concentration of a compound in the liquid phase is, in the stationary state, in equilibrium with its concentration in the gas phase through its partial pressure. In anaerobic digestion, compounds are first formed in the liquid phase before being transferred to the gas phase. However, this transfer of matter is very often a limiting phenomenon influencing the performance of the reactors. Compounds such as methane and hydrogen, which are not very soluble, can then become supersaturated. The most common way to define liquid-gas transfers is the Whitman double film theory. In the present model, it is considered that liquid-gas equilibria are established through this double film only by molecular diffusion.

2. Material and Methods

2.1 Structure of the Model

We considered the degradation of organic matter as a whole as a succession of three steps (Hydrolysis, Acidogenesis, Methanogenesis) where the products formed serve as a substrate for the next step.

The first step is hydrolysis where the solid organic matter S_0 is hydrolyzed into soluble compounds (protein, lipids, ...), all assimilated to a substrate S_1 . Then, substrate S_1 is degraded into Volatile Fatty Acids (substrate S_2) and CO_2 by the action of acidogenic bacteria X_1 . In the third step, substrate S_2 is consumed by the methanogenic bacteria X_2 to produce mainly methane CH_4 and carbon dioxide CO_2 .

We represent this process in a macroscopic way by the following reaction scheme.^[7,8]

Acidogenesis reaction rate: $r_A = \mu_1 [X_1]$,

Reaction rate methanogenesis: $r_M = \mu_2 [X_2]$,

k_i : Coefficients of yield ($i = 1, 2, 3, 4, 5, 6$),

k_h : Hydrolysis constant.

2.2. Equations governing the decomposition process of organic matter

The material balances on the fed reactors are based on the law of conservation of mass, which takes into account the incoming and outgoing material flows, as well as biological reactions. Thus, the evolution of the mass of a constituent is given by the relation:

$$\text{Input} + \text{Production} = \text{Output} + \text{Accumulation}$$

$$Q_{in} C_{in} + rV = Q_{out} C_{out} + \frac{d(VC)}{dt} \quad (4)$$

Boundary conditions

Perfectly agitated continuous reactor: $C_{out} = C$

Feeding and Racking: $Q_{in} = Q_{out} = Q$

Fig. 2 Simplified diagram of a continuous reactor of volume V .

Thus, Equation (1) becomes successively:

$$V \frac{dC}{dt} = Q(C_{in} - C) + rV \quad (5)$$

$$\frac{dC}{dt} = \frac{Q}{V}(C_{in} - C) + r \quad (6)$$

By posing $D = \frac{Q}{V}$, we obtain the equation governing the anaerobic digestion process in a continuous reactor:

$$\frac{dC}{dt} = D(C_{in} - C) + r \quad (7)$$

By applying Equation (7), for microorganisms of concentration $[X]$ we obtain the fundamental growth equation called microorganism growth kinetics:

$$\frac{d[X]}{dt} = D([X_{in}] - [X]) + \mu[X] \quad (8)$$

By applying Equation (7), for substrates of concentration $[S]$ we obtain the fundamental consumption equation called substrate consumption kinetics:

$$\frac{d[S]}{dt} = D([S_{in}] - [S]) - \frac{1}{Y}\mu[X] \quad (9)$$

μ : Specific rate or speed of growth.

Y : Biomass yield.

By applying the growth kinetics obtained in Equation (8) to the microorganisms X_1 and X_2 we obtain the following equations:

$$\frac{d[X_1]}{dt} = (\mu_1 - D)[X_1] \quad (10)$$

$$\frac{d[X_2]}{dt} = (\mu_2 - D)[X_2] \quad (11)$$

By applying the substrate consumption or utilization kinetics obtained in Equation (9) to substrates S_0 , S_1 , and S_2 we obtain the following equations:

$$\frac{d[S_0]}{dt} = D([S_0^{in}] - [S_0]) - k_h[S_0] \quad (12)$$

$$\frac{d[S_1]}{dt} = D([S_1^{in}] - [S_1]) + k_h[S_0] - k_1\mu_1[X_1] \quad (13)$$

$$\frac{d[S_2]}{dt} = D([S_2^{in}] - [S_2]) + k_2\mu_1[X_1] - k_4\mu_2[X_2] \quad (14)$$

k_i : Coefficients of yield ($i = 1, 2, 4$).

D : Dilution rate.

The growth rates used are those of Monod^[9] and Haldane^[10] for the respective acidogenesis and methanogenesis steps:

$$\mu_1 = \mu_{1max} \frac{[S_1]}{[S_1] + K_{S1}} \quad (15)$$

$$\mu_2 = \mu_{2max} \frac{[S_2]}{[S_2] + K_{S2} + \frac{([S_2])^2}{K_{12}}} \quad (16)$$

$$P_{CO_2} [k_{La}([CO_2L] - K_H P_{CO_2}) + k_6\mu_2[X_2]] = k_{La}P_T([CO_2L] - K_H P_{CO_2}) \quad (22)$$

$$k_{La}K_H P_{CO_2}^2 - P_{CO_2}(k_{La}[CO_2L] + k_6\mu_2[X_2] + k_{La}K_H) + k_{La}[CO_2L]P_T = 0 \quad (23)$$

Q_{in} : Input Flow [m^3/s]

Q_{out} : Output flow rate [m^3/s]

C_{in} : Input concentration [mol/m^3]

V : reactor volume [m^3]

C : Concentration inside the reactor [mol/m^3]

r : Biochemical reaction rate.

2.3 Dynamics of carbon dioxide in the liquid phase

Anaerobic digestion is a controlled biological decomposition process that takes place without oxygen and generates both, biogas (methane, carbon dioxide, dihydrogen) and digestate. But in reality, the products such as methane, carbon dioxide, and dihydrogen are obtained first in their soluble form before they are transferred to the gas phase by the phenomenon of liquid-gas transfer. Thus, according to Equations (2) and (3), the dynamics of carbon dioxide in the liquid phase are given by the following relation:

$$\frac{d[CO_2L]}{dt} = k_3\mu_1[X_1] + k_5\mu_2[X_2] \quad (17)$$

2.4 Molar composition of biogas

The CH_4 and CO_2 contents of the biogas are calculated from the outputs q_{CH_4} and q_{CO_2} of the model. Since the degradation products are obtained first in their soluble form, the gaseous products are obtained by transfer from the liquid to the gaseous phase. Since methane is not very soluble and is instantaneously found in the gaseous phase, we have chosen to represent only the transfer of carbon dioxide from the liquid to the gaseous phase.

The molar flow of methane is directly related to the growth of the methanogenic bacterial population and is defined by:

$$q_{CH_4} = k_6\mu_2[X_2] \quad (18)$$

As for the molar flow of carbon dioxide, it is obtained from the liquid-gas transfer rate based on the two-film theory. Its expression is given by the relation:

$$q_{CO_2} = k_{La}([CO_2L] - K_H P_{CO_2}) \quad (19)$$

The partial pressure of carbon dioxide is calculated from the flow rates of different gases and the total pressure (P_T). According to Dalton's law, we obtain:

$$P_{CO_2} = \frac{q_{CO_2}}{q_{CO_2} + q_{CH_4}} P_T \quad (20)$$

By combining Equations (18), (19), and (20), we obtain successively:

$$P_{CO_2} = \frac{k_{La}([CO_2L] - K_H P_{CO_2})}{k_{La}([CO_2L] - K_H P_{CO_2}) + k_6\mu_2[X_2]} P_T \quad (21)$$

$$K_H P_{CO_2}^2 - P_{CO_2} \left([CO_2L] + \frac{k_6}{k_{La}} \mu_2 [X_2] + K_H P_T \right) + [CO_2L] P_T = 0 \quad (24)$$

$$\text{Then, } \Delta = \left([CO_2L] + \frac{k_6}{k_{La}} \mu_2 [X_2] + K_H P_T \right)^2 - 4 K_H P_T [CO_2L] \quad (25)$$

$$\Delta = ([CO_2L] + K_H P_T)^2 + 2 \frac{K}{k_{La}} \mu_2 [X_2] ([CO_2L] + K_H P_T) + \left(\frac{k_6}{k_{La}} \mu_2 [X_2] \right)^2 - 4 K_H P_T [CO_2L] \quad (26)$$

$$\Delta = ([CO_2L] - K_H P_T)^2 + 2 \frac{k_6}{k_{La}} \mu_2 [X_2] ([CO_2L] + K_H P_T) + \left(\frac{k_6}{k_{La}} \mu_2 [X_2] \right)^2 \quad (27)$$

This discriminant being positive, then Equation (24) admits two solutions, the greater of which is greater than the total pressure; which is not physically admissible, so we retain the following solution:

$$P_{CO_2} = \frac{[CO_2L] + \frac{k_6}{k_{La}} \mu_2 [X_2] + K_H P_T - \sqrt{\Delta}}{2 K_H} \quad (28)$$

The proportions of methane and carbon dioxide in the gas mixture are given:

$$\% CH_4 = \frac{q_{CH_4}}{q_{CO_2} + q_{CH_4}} \times 100 \text{ and } \% CO_2 = \frac{q_{CO_2}}{q_{CO_2} + q_{CH_4}} \times 100$$

By replacing q_{CH_4} and q_{CO_2} by their respective expressions, we can obtain:

$$\% CH_4 = \frac{k_6 \mu_2 [X_2]}{k_6 \mu_2 [X_2] + k_{La} ([CO_2L] - K_H P_{CO_2})} \times 100 \quad (29)$$

$$\% CO_2 = \frac{k_{La} ([CO_2L] - K_H P_{CO_2})}{k_6 \mu_2 [X_2] + k_{La} ([CO_2L] - K_H P_{CO_2})} \times 100 \quad (30)$$

2.5 Modeling the influence of temperature

The temperature inside the digester is one of the main conditions for the good functioning of methanization. It must be within very precise temperature ranges. Indeed, a too-high temperature will lead to the death of the micro-organisms necessary for the production of biogas while a too-low temperature will slow down the methanization process. This is why this work has focused on the study of the influence of temperature from a numerical model. In order to have the temperature as input in this model, we used the Ratkowsky formula which gives the maximum bacterial growth rate as a function of temperature.

Indeed, in anaerobic digestion all measurable factors that influence the growth rate (μ) are independent and

multiplicative:

$$\mu = f(\text{temperature}) \times f(\text{pH}) \times f(\text{others}_1) \times \dots \times f(\text{others}_n) \quad (31)$$

The effect of each factor on the growth rate can be represented by a fraction of the maximum growth rate:

$$\gamma(f_i) = \frac{\mu(f_i)}{\mu_{opt}} \quad (32)$$

The maximum rate of bacterial growth is given by:

$$\mu_{max} = \mu_{opt} \prod_{i=1}^n \gamma(f_i) \quad (33)$$

The f_i represent the environmental factors influencing the process such as temperature, water content, pH, etc. Using Equations (32) and (33) in this work where we study the influence of temperature, we obtain:

$$\mu_{max} = \mu(T). \quad (34)$$

Thus Ratkowsky *et al.* developed the square root model which was later extended. We considered the Ratkowsky square root model because it is the most appropriate for describing the maximum growth rate as a function of temperature. Its expression is:

$$\mu_{max} = [b(T - T_{min})]^2 (1 - \exp[c(T - T_{max})]) \quad (35)$$

where b and c are constant model parameters obtained by regression, T is the temperature in °C, T_{min} is the minimum growth temperature and T_{max} is the maximum growth temperature.

2.6 Differential equations of the model.

We obtain a model composed of six first-order coupled ordinary fundamental differential equations of the state vector $Y = [S_0 \ X_1 \ S_1 \ X_2 \ S_2 \ CO_2L]^T$ and two major output variables $\% CH_4$ and $\% CO_2$.

$$\left\{ \begin{array}{l} \frac{d[S_0]}{dt} = D([S_0^{in}] - [S_0]) - K_h[S_0] \\ \frac{d[X_1]}{dt} = (\mu_1 - D)[X_1] \\ \frac{d[S_1]}{dt} = D([S_1^{in}] - [S_1]) + k_h[S_0] - k_1\mu_1[X_1] \\ \frac{d[X_2]}{dt} = (\mu_2 - D)[X_2] \\ \frac{d[S_2]}{dt} = D([S_2^{in}] - [S_2]) + k_2\mu_1[X_1] - k_3\mu_2[X_2] \\ \frac{d[CO_2L]}{dt} = k_3\mu_1[X_1] + k_5\mu_2[X_2] \\ \% CH_4 = \frac{k_6\mu_2[X_2]}{k_6\mu_2[X_2] + k_{La}([CO_2L] - K_H P_{CO_2})} \times 100 \\ \% CO_2 = \frac{k_{La}([CO_2L] - K_H P_{CO_2})}{k_6\mu_2[X_2] + k_{La}([CO_2L] - K_H P_{CO_2})} \times 100 \\ \mu_1 = [b_1(T - T_{min})]^2 (1 - \exp[c_1(T - T_{max})]) \frac{[S_1]}{[S_1] + K_{S_1}} \\ \mu_2 = [b_2(T - T_{min})]^2 (1 - \exp[c_2(T - T_{max})]) \frac{[S_2]}{[S_2] + K_{S_2} + \frac{([S_2])^2}{K_{12}}} \end{array} \right. \quad (36)$$

2.6.1 Existence and uniqueness of solutions of the system (36)

The present model is a system of non-linear, non-autonomous first-order differential equations of the form: $U'(t) = F(U(t), t)$, where F is a continuous function of $\mathbb{R}_+^6 \times \mathbb{R}_+$ in $\mathbb{R}^6$:

$$F(t) = \begin{pmatrix} D([S_0^{in}] - [S_0]) - K_h[S_0] \\ (\mu_1 - D)[X_1] \\ D([S_1^{in}] - [S_1]) + k_h[S_0] - k_1\mu_1[X_1] \\ (\mu_2 - D)[X_2] \\ D([S_2^{in}] - [S_2]) + k_2\mu_1[X_1] - k_3\mu_2[X_2] \\ k_3\mu_1[X_1] + k_5\mu_2[X_2] \end{pmatrix};$$

$$U(t) = \begin{pmatrix} [S_0(t)] \\ [X_1(t)] \\ [S_1(t)] \\ [X_2(t)] \\ [S_2(t)] \\ [CO_2L(t)] \end{pmatrix}$$

F being of class C^∞ with respect to U , thus locally lipschitzian with respect to U on $\mathbb{R}_+^6$. Moreover, F is continuous with respect to t , which implies the existence and uniqueness of a maximal solution of the Cauchy problem associated with the nonlinear differential system on $[0; t_{max}]$, where $t_{max} > 0$, for an initial condition $U_0 \in \mathbb{R}_+^6$. Biologically, the only significant solutions are the positive ones; this is why we have limited our study on $\mathbb{R}_+^6$.

2.6.2 Study of the model equilibrium and stability of the equilibrium states.

Studying the equilibrium of the model is the same as studying the equilibrium of the system of fundamental equations of the model. We will therefore look for the points where the first derivatives are zero. Thus, we obtain the following relation:

$$\begin{cases} \frac{d[S_0]}{dt} = D([S_0^{in}] - [S_0]) - K_h[S_0] & = 0 \\ \frac{d[X_1]}{dt} = (\mu_1 - D)[X_1] & = 0 \\ \frac{d[S_1]}{dt} = D([S_1^{in}] - [S_1]) + K_h[S_0] - k_1\mu_1[X_1] & = 0 \\ \frac{d[X_2]}{dt} = (\mu_2 - D)[X_2] & = 0 \\ \frac{d[S_2]}{dt} = D([S_2^{in}] - [S_2]) + k_2\mu_1[X_1] - k_3\mu_2[X_2] & = 0 \end{cases} \quad (37)$$

From the first equation of the system (37) we deduce:

$$D([S_0^{in}] - [S_0]) - K_h[S_0] = 0 \Leftrightarrow [S_0] = \frac{D}{K_h + D} [S_0^{in}]$$

The first equation of the system (36) depends only on the variable $[S_0]$ and $[S_0]$ converges globally to its equilibrium $[S_0^\theta] = \frac{D}{K_h + D} [S_0^{in}]$.

At $[S_0]$ equilibrium, the last four equations of the model reduce to the AM2 model in the case where $\alpha = 1$.

$$\begin{cases} \frac{d[X_1]}{dt} = (\mu_1 - D)[X_1] \\ \frac{d[S_1]}{dt} = D([S_1^{in}] - [S_1]) - k_1\mu_1[X_1] \\ \frac{d[X_2]}{dt} = (\mu_2 - D)[X_2] \\ \frac{d[S_2]}{dt} = D([S_2^{in}] - [S_2]) + k_2\mu_1[X_1] - k_3\mu_2[X_2] \end{cases} \quad (38)$$

$$\text{where, } [S_1^{\theta in}] = [S_1^{in}] + \frac{K_h}{K_h + D} [S_0^{in}]$$

(39)

To reach equilibrium $E_1 = ([X_1^\theta], [S_1^\theta], [X_2^\theta], [S_2^\theta])$ of the AM2 model (system 38) corresponds to an equilibrium $E_2 = ([S_0^\theta], [X_1^\theta], [S_1^\theta], [X_2^\theta], [S_2^\theta])$ of the present model. Furthermore, their local stability is deduced from that of the corresponding E_1 equilibria of the AM2 model. The analysis of the equilibrium and stability of the equilibrium points of the AM2 model has been done in Refs. [13] and [14]. The following result is obtained.

Proposition: The equilibrium points of the AM2 model are given by:

- i) $E_0 = ([S_0^\theta], 0, [S_1^{\theta in}], 0, [S_2^{\theta in}])$ which still exists.
- ii) $E_1^i = ([S_0^\theta], 0, [S_1^{\theta in}], [X_2^i], \lambda_2^i)$ which exists if and only if $S_2^{in} > \lambda_2^i$, where $[X_2^i] = \frac{1}{k_3}([S_2^{in}] - \lambda_2^i)$ and λ_2^i ($i = 1, 2$) solutions of the equation $\mu_2([S_2]) = D$.
- iii) $E_2^0 = ([S_0^\theta], [S_1^\theta], \lambda_1, 0, [S_2^{\theta in}])$, which exists if and only if $[S_1^{\theta in}] > \lambda_1$.
- iv) $E_2^i = ([S_0^\theta], [S_1^\theta], \lambda_1, [X_2^i], \lambda_2^i)$ which exists if and only if $[S_1^{\theta in}] > \lambda_1$.

2.6.3 Algorithm of numerical resolution.

In order to numerically solve the system of differential equations of the present model, we have reformulated this system of equations as follows in Equation (40):

$$\frac{dY}{dt} = F(Y, t); Y = [[S_0] \ [X_1] \ [S_1] \ [X_2] \ [S_2] \ [CO_2L]]^T; F = [F_1 \ F_2 \ F_3 \ F_4 \ F_5 \ F_6]^T$$

$$\begin{cases} F_1(Y, t) = D([S_0^{in}] - [S_0]) - K_h[S_0] \\ F_2(Y, t) = (\mu_1 - D)[X_1] \\ F_3(Y, t) = D([S_1^{in}] - [S_1]) + k_h[S_0] - k_1\mu_1[X_1] \\ F_4(Y, t) = (\mu_2 - D)[X_2] \\ F_5(Y, t) = D([S_2^{in}] - [S_2]) + k_2\mu_1[X_1] - k_3\mu_2[X_2] \\ F_6(Y, t) = k_3\mu_1[X_1] + k_5\mu_2[X_2] \end{cases} \quad (40)$$

For the numerical resolution of the model, programming under the SCILAB environment has been developed and implemented for the simulation of the digester operation. We used the ordinary differential equations (ODE) solver and the graphical interface under SCILAB for the visualization of the responses. The results representing the numerical solution of the ordinary differential equations of the anaerobic digestion system were plotted using the graphical interface.

The algorithm used for the numerical solution of the system of differential equations is as follows:

- i) Programming the $F(Y, t)$. function in SCILAB
- ii) Definition of initial conditions Y_0 .
- iii) Definition of the initial and final times t_0 and t_n .
- iv) Automatic choice of discretization and adapted scheme.
- v) Calculation of the solution Y at the final time t_n : $Y = \text{ode}(Y_0, t_0, t_n, F)$
- vi) Programming of production graphic outputs.
- vii) Programming the calculation and display of CH_4 and CO_2 contents.

2.7 Experimental data

In order to numerically solve the first-order differential equation system, the initial conditions, which are estimates of the initial quantities of substrate and bacteria concentrations at bioreactor start-up, must be provided. The different values of the initial conditions are taken from the literature^[15] and are presented as follows: $[S_0](0) = 0 \text{ g/L}$; $[S_1](0) = 10 \text{ g/L}$; $[S_2](0) = 2 \text{ g/L}$; $[X_1](0) = 0,4 \text{ g/L}$; $[X_2](0) = 0,01 \text{ g/L}$; $[\text{CO}_2\text{L}](0) = 0$; $D = 0$.

An extensive review of the literature has provided us with estimates of some parameters of this model. The others were obtained by fitting the model to obtain consistent results. The different values of the Ratkowsky parameters are presented as follows:^[16]

$b_1 = 0.041$; $b_2 = 0.00254$; $c_1 = 0.161$; $c_2 = 0.161$; $T_{\min} = 2^\circ\text{C}$ and $T_{\max} = 43.7^\circ\text{C}$.

The values of the kinetic, equilibrium and transfer parameters are presented in Table 1.

3. Results and Discussions

3.1 Biogas production kinetics

The biogas volume is an important parameter for the control and monitoring of the anaerobic digestion process because it integrates the other process parameters. Simulation results, allowing us to graphically visualize the temporal evolution of the predicted cumulative volume and biogas flow rate, are shown in Figs. 3 and 4, respectively.

Fig. 3 Simulated cumulative biogas volume.

Fig. 4 Simulated biogas flow rate.

Table 1. Kinetic, equilibrium, and transfer parameters.^[17-21]

Parameters	Significance	Values	Units
k_1	Substrate degradation yield S_1 .	50	(g/g)
k_2	Substrate production yield S_2	50	(g/g)
k_3	The production yield of CO_2 L	35	(g/g)
k_4	Substrate degradation yield S_2	35	(g/g)
k_5	The production yield of CO_2 L	15	(g/g)
k_6	The production yield of CH_4	75	(L^2/mg)
K_{S_1}	Half-saturation constant associated with S_1 .	35	(mg/L)
K_{S_2}	Half-saturation constant associated with S_2	4	(mg/L)
k_h	Hydrolysis constant	0.5	(d^{-1})
K_{I2}	Inhibition constant associated with the substrate S_2 .	170	(mg/L)
$\mu_{1\max}$	Maximum growth rate associated with X_1 .	0.13	(d^{-1})
$\mu_{2\max}$	Maximum growth rate associated with X_2 .	0.23	(d^{-1})
P_T	Total gas pressure	1	(Bar)
K_H	Henry's constant	1	($\text{mmol.L}^{-1}.\text{atm}^{-1}$)
k_{La}	Gas/liquid volume transfer coefficient	0.078	(d^{-1})

In Fig. 3, we can see that the cumulative methane and carbon dioxide production kinetics are divided into two main phases: a lag phase (1 to 14 days) followed by the exponential growth phase (15 to 36 days). During this last phase, the multiplication of microorganisms is important, which leads to the important production of biogas. This is due to a degradation of the organic matter that increases significantly with the initial concentration of microorganisms. These results show a slight dominance of methane in the gas mixture.

In Fig. 4, we witness a continuously increasing production of methane and carbon dioxide that starts from the fifth day of the process reaching maximum values of 6.4 L/d and 4.1 L/d respectively at day 33. Then, we register a continuous decrease in methane and carbon dioxide production which become almost null on the 58th day. This is explained by the depletion of organic matter and the consequence of the depletion of Volatile Fatty Acids. We note a predominance of methane in the gas mixture.

Moreover, the molar composition of the simulated biogas is as shown in Fig. 5. We record a continuous rise of the proportion of carbon dioxide in the mixture until the 5th day, then a slight decrease of this proportion until the 60th day of fermentation. On the other hand, the proportion of methane varies in the opposite direction.

These results show a slight dominance of methane in the last days of the process, which gives the simulated biogas a combustible character with percentages of the same order of magnitude as those given in the scientific literature.

Fig. 5 Molar composition of the gas mixture as a function of time.

3.2 Influence of the temperature

To study the effect of temperature, we varied this parameter from 20 °C to 40 °C with a step of 5 °C. Fig. 6 shows the evolution of the cumulative biogas volume as a function of temperature. As shown in this figure, the simulated cumulative biogas volume increases as the temperature increases in the range of 20 °C-35 °C and peaks at 35 °C. However, this volume decreases as the temperature increases beyond this optimum value.

Knowing that the optimal temperature for an anaerobic digestion system in a mesophilic regime is around 37 °C, we can say that the results obtained with this present model are in accordance with the experimental results obtained by several

authors^[22-23] and in particular Batstone *et al.* who proved on an experimental scale that the increase of the temperature above the optimum induces a decrease of the degradation rates and a decrease of the yields due to an increase of the energy necessary for the renewal and the cellular maintenance. The same authors proved that the variation of the temperature inside the reactors induces a modification of the metabolic ways and the outputs due to variations of the thermodynamic conditions and the bacterial populations, and that, the increase of the temperature induces an increase in the rate of mortality of the bacteria because of phenomena of cellular lysis and modified cellular maintenance.

Fig. 6 Cumulative volume of biogas as a function of temperature.

According to Arrhenius' law, the rate of reactions that take place in methanization must increase with temperature. However, the literature also reports contradictory results. Thus, according to Parkin & Owen,^[24] an increment from 35 to 45 °C does not change the gas production, while a change from 35 to 50 °C generates a decrease in methane production. Thus, we can note that the microorganisms involved in the methanization process present a very large variety. This variety is found in the thermal optima which are situated in a range of temperatures going from 35 °C to 65 °C according to the type of microorganism. The operation at high temperatures allows for improvement in the hydrolysis speed and the elimination of the organic matter. However, the process is less stable due to the rapid production of volatile fatty acids and inhibiting substances such as ammonium, among others.

Figure 7 shows the variation of the molar composition of the biogas as a function of temperature. We note that at a temperature of 20 °C the average proportion of methane is higher than that of carbon dioxide and this observation was made for temperatures of 25 °C, 30 °C, 35 °C, and 40 °C. Moreover, we note a decrease in the proportion of methane at the temperature of 30 °C from 61.52% to 50.72%, then a progressive increase to 61% at a temperature of 35 °C. This proportion drops again to 53.94% at a temperature of 40°C. Conversely, we note an increase in the average proportion of carbon dioxide from 38.48% to 49.28%, then a decrease to 39% at the temperature of 35 °C. These results clearly show the predominance of methane in the gas mixture, which gives

Fig. 7 Gas mixture composition as a function of temperature.

the simulated biogas the "combustible" character with percentages of the same order of magnitude as those given in the scientific literature. From the analysis of Figs. 6 and 7, it is clear that the numerical values obtained are in agreement with the experimental data provided by the literature.

In view of the above, we can say that the variation of the temperature inside the digesters has a great influence on the production of biogas, both quantitatively and qualitatively. This variation affects the liquid/gas equilibrium and the equilibrium of the chemical species present in the digestion media, which leads to a huge variation in its molar composition.

3.3 Model Validation

During the validation of the present model, the accuracy of the model was tested using external experimental data by applying the statistical parameters of residual root mean square error in prediction (RMSE) and relative residual root mean square error in prediction (rRMSE), which is a normalized RMSE

using the mean value of measured experimental values. The least squares regression was performed by minimizing the residual sum of squares (RSS):

$$RSS = \sum_{i=1}^N (y_i - \tilde{y}_i)^2 \quad (41)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \tilde{y}_i)^2} \quad (42)$$

$$rRMSE = \frac{RMSE}{\bar{y}} \quad (43)$$

where, y_i is the value of measurement number i , $\tilde{y}_i$ is the corresponding predicted value, $\bar{y}$ is the average value of the measurements, N is the number of measurements, The input conditions used^[25] are:

$[S_0^{in}] = 161 \text{ g/L}$; $[S_1^{in}] = 0 \text{ g/L}$; $[S_1] = 0 \text{ g/L}$; $[S_2] = 0 \text{ g/L}$; $[X_1^{in}] = 64 \text{ g/L}$; $[X_2^{in}] = 12 \text{ g/L}$; $q_{CO_2}(0) = 0$; $q_{CH_4}(0) = 0$; $D = 0.5$.

From the analysis of Fig. 8, it appears that there is a good agreement between the curves obtained on the evolution of the cumulative volume of biogas at certain levels.

Fig. 8 Cumulative volume of biogas predicted and obtained experimentally [25].

Fig. 9 Quality adjustment between experimental and simulated values.

The validation results were very interesting, as the model tended to overestimate the biogas production. On the other hand, it showed a relatively fine accuracy at the beginning and toward the end of the digestion. The rRMSE value obtained is 18.8%, which corresponds to a model error of 4.23 (L). The coefficient of determination R^2 is 0.96 (Fig. 9); this shows a higher level of correlation compared to the relatively low accuracy of the model.

Considering the results given by the different simulations under the SCILAB environment and in comparison, with the results from the scientific literature, we can say that the

proposed model performed well for the prediction of biogas production.

3.4 Model sensitivity

In order to be able to judge the influence of a few parameters on the simulations of the present model, it is essential to know the sensitivity of the model with respect to these parameters. For this purpose, we will carry out several series of simulations by varying certain parameters independently. The conditions of implementation are given in Table 2:

Table 2. Conditions implemented for the sensitivity of the model.

Simulations	Parameters	Symbols	Basic values	Sensitivity values
1	Transfer coefficient	kLa	0.078 j^{-1}	$\times (0.1; 0.5; 2; 10)$
2	The initial concentration of methanogenic bacteria	X_2^{in}	0.01 g/L	$\times (0.1; 0.5; 2; 10)$

Fig. 10 Sensitivity of the transfer coefficient.

Fig. 11 Sensitivity of the initial concentration of methanogenic bacteria.

3.4.1 Sensitivity of the transfer coefficient

The transfer coefficient (kLa) is the most important factor when simulating transfers between liquid and gaseous phases. For given biological kinetic parameters, the transfer kinetics of gaseous compounds from the liquid phase is mainly influenced by this parameter. Fig. 10 illustrates the influence of kLa on biogas production. We notice clearly in this figure that the transfer coefficient has a significant influence on biogas production. The higher this coefficient, the higher the maximum production achieved.

3.4.2 Sensitivity of the initial concentration of methanogenic bacteria.

The results obtained (Fig. 11) show that the initial concentration of methanogenic bacteria has an influence on the degradation of substrates and consequently on the production of biogas. The kinetics of biogas production increases progressively as the initial concentration of methanogenic bacteria rises. Then, the maximum biogas production remains almost constant for the initial concentrations of 0.005 g/L, 0.01 g/L, 0.02 g/L, and 0.1 g/L of methanogenic bacteria.

3.5 Limitations of the model

The limitations of the present model lie in the kinetic and phase transfer parameters that influence the results of the different simulations. These parameters are very difficult to determine due to the complexity of the biochemical mechanisms and the experimental conditions specific to each bioreactor. For the present model, these parameters have been estimated from the values published in the literature and have been obtained under experimental conditions that are not all similar.

4. Conclusion and Prospects

Experimentation is the best solution to define methanization processes, unfortunately, it remains very expensive. For this purpose, we have proposed a mathematical model governing the physicochemical and biological phenomena of these processes. This model highlights the influence of the internal temperature of the digesters on the production of biogas. From the analysis of the simulation results, it appears that the numerical results are satisfactory with respect to the experimental data. Moreover, the cumulative volume of simulated biogas increases as the temperature rises in a range of 20 °C-35 °C and reaches its peak at 35 °C. However, this volume decreases when the temperature rises above this optimal value. It appears from the present study that the optimal methanation temperature depends on the type of microorganism and is between 35-38 °C for continuous digesters in a mesophilic regime.

We then plan to determine, through experimentation under precise conditions, the kinetic and phase transfer parameters in order to study the combined influence of several operational parameters on biogas production.

Acknowledgments

This work was mutually supported by the authors themselves. No international or national agency funded this work. No funding for this study.

Conflict of Interest

There is no conflict of interest.

Supporting Information

Not Applicable.

Nomenclature and Description of Parameters

Parameters	Description	Units
k_1	Substrate degradation yield S_1 .	(g/g)
k_2	Substrate production yield S_2	(g/g)
k_3	Production yield of CO_2 L	(g/g)
k_4	Substrate degradation yield S_2	(g/g)
k_5	Production yield of CO_2 L	(g/g)
k_6	Production yield of CH_4	(L ² /mg)
$[S_0]$	Initial substrate concentration	g/L
$[S_1]$	Concentration of soluble substrate	g/L
$[S_2]$	Concentration of Volatile Fatty Acids	g/L
$[X_1]$	Concentration of acidogenic microorganisms	g/L
$[X_2]$	Concentration of methanogenic microorganisms	g/L
$[CO_2L]$	Concentration of CO_2 in the liquid phase.	g/L
D	Dilution rate	d ⁻¹
K_{S_1}	Half-saturation constant associated with S_1 .	(mg/L)
K_{S_2}	Half-saturation constant associated with S_2	(mg/L)
k_h	Hydrolysis constant	(d ⁻¹)
K_{I2}	Inhibition constant associated with the substrate S_2 .	(mg/L)
μ_{1max}	Maximum growth rate associated with X_1 .	(d ⁻¹)
μ_{2max}	Maximum growth rate associated with X_2 .	(d ⁻¹)
P_T	Total gas pressure	(Bar)
P_{CO_2}	Partial pressure of CO_2	(Bar)
K_H	Henry's constant	(mmol L ⁻¹ atm ⁻¹)
k_{La}	Gas/liquid volume transfer coefficient	(d ⁻¹)

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