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New methodology for calculating the production of biogas in livestock wastewater treatment systems

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ABSTRACT

In this work, a modelling and numerical simulation proposal has been developed with a free open-source software, Scilab. The learning proposal consists of the simulation of an anaerobic biodigester under continuous and discontinuous loading with an AM2 mathematical model based on two reactions, acidogenesis-acetogenesis, considering a Monod-type growth, and methanogenesis, with a Haldane-type growth. Anaerobic digestion has become a successful process for the stabilisation of wastewater with high organic load. The aim of this proposal is to be used in the practical training activities to be developed by the student in the context of some of the subjects of the University Degrees and Masters with competences in the area of environmental technology. In the simulations, the proposed model has proved to be an effective tool for the simulation of the anaerobic digestion process, it has proved to be an efficient system to reduce the organic load in wastewater and it is versatile as it allows to modify the design, quickly, depending on the future needs of the student or teacher that can be used to understand and learn the proposed objective.

Keywords: Numerical methods; Anaerobic digestion; Anaerobic digestion; Model; Scilab

1. Introduction

Anaerobic digestion has become a successful process for the stabilisation of wastewater with high organic load, and it is important to understand the various factors that affect bioreactor design. Also, anaerobic treatment systems are natural processes that take place in areas where free oxygen is not available and are ideal for the treatment of highly biodegradable wastes. Anaerobic digestion has become more popular in recent years, mainly due to its ability to generate energy from waste [1]. Advances in microbial ecology methodologies in recent decades have resulted in tools to qualify and quantify microbially driven systems, allowing theorists to better test hypotheses, resulting in the potential for better engineering design and operation of biological processes [2].

The main objective of this work is a simple proposal for modelling and numerical simulation with SCILAB, for learning the continuous and discontinuous dynamics of biological digesters with an AM2 mathematical model for wastewater treatment, due to the high cost that must be faced when implementing a facility of this type [3–5]. For this reason, several mathematical models have been developed for simulation, the usefulness of which depends on the objective and complexity of the work.

The Scilab software, which is free and open source, has been chosen to carry out the simulation. This software is oriented towards numerical computation, especially for

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scientific and engineering applications. It can be used as a simple matrix calculator, but its main interest lies in its hundreds of general-purpose and specialised functions, as well as in its possibilities for graphical visualisation. Several authors have chosen this program because many examples of ready-made and tested programs can be found at [6–10].

Therefore, it is of interest to develop learning strategies, based on ICTs, which help students, of the degrees and masters of the area with competences in environmental technologies, to learn and understand the evolution of the relevant variables in the operation of anaerobic bioreactors, also being useful for the estimation of the biogas generation potential and its valuation as an energy vector [8,10]. This work is carried out within the framework of the Educational Innovation Projects for Interdisciplinary Training (PIEFI) – Line 3. Contents and programmes of teaching in the project "Laboratories as working environments for active and collaborative learning through the design, development, construction, use and redesign of equipment and devices for their application in practices" (PIE 2022–60) of the University of Las Palmas de Gran Canaria (ULPGC).

2. Theoretical foundations of anaerobic digestion

Anaerobic digestion, also called biogas production, is a microbiological process that occurs spontaneously in nature in the absence of oxygen. It breaks down organic matter into simpler compounds, which are transformed into volatile fatty acids, which are the main intermediates and modulators of the process to obtain a mixture of gases called biogas, this process is carried out by the action of a group of specific microorganisms working in sequences [4,11].

Anaerobic digestion is a very complex process due to the high number of biochemical reactions taking place and the number of bacteria involved. In fact, many of these reactions occur simultaneously [4,11]. Digestion can be grouped into three main stages: hydrolysis, acid formation and methanogenesis, which will be explained in the section on phases of anaerobic digestion. The higher the number of stages considered in the mathematical model, the higher the complexity of the model, but at the same time the better the representativeness of the process [4,11].

As a complex process, modelling of anaerobic digestion improves the understanding of the process and allows the formulation or validation of certain hypotheses regarding the process itself. A mathematical model allows to predict the behaviour of this complex process when subjected to different conditions of its manipulable variables such as temperature, concentration, composition and flow of the input substrates, pH level, oxygenation, etc. and thus reduces the possible complications that can be obtained when the process is carried out [1].

2.1. Model AM2

As for the mathematical modelling of the anaerobic digestion process, the AM2 model proposed by Bernard in 2001 is designed to use as substrate wastewater containing soluble, carbohydrate-based organic matter, so that the hydrolysis step is irrelevant. In this model it only considers two limiting reactions, the acidogenesis of the substrate from the influent (S_1) and the methanegenesis of the volatile fatty acids (S_2), obtained as a product in the first of the reactions [4,12]. It is intended for analytical and control applications or instrumentation development.

2.2. Components

In the AM2 mathematical model, at least four components are required to describe what happens in a digester, the substrate, which is the component that serves as food for the biomass, S_1 and S_2, and the biomass, which is the culture of microorganisms that feed on the biodegradable organic matter, X_1 and X_2.

2.3. Biological processes in the digester

The model considers only two limiting steps, acidogenesis and methanogenesis. First reaction: acidogenesis of the substrate supplied by the influent.

$$\alpha_1 S_1 \xrightarrow{\mu_1} X_1 + \alpha_2 S_2 + \alpha_3 CO_2 \tag{1}$$

where S_1 is the organic substrate in the influent, X_1 is the population of acidogenic bacteria and α_i are the stoichiometric coefficients of each species.

The kinetics used is the Monod model.

$$\mu_1 = \mu_{max1} \cdot \frac{S_1}{K_S + S_1} \tag{2}$$

where μ_{max1} is the maximum growth and K_s is the Michaelis–Menten constant. Second reaction: volatile fatty acid methanogenesis.

$$\alpha_1 S_2 \xrightarrow{\mu_2} X_2 + \alpha_2 CH_4 + \alpha_3 CO_2 \tag{3}$$

where S_2 are the volatile fatty acids obtained from acidogenesis, X_2 is the population of methanogenic bacteria and α_i are the stoichiometric coefficients of each species.

The kinetics used is the Haldane model.

$$\mu_2 = \mu_{max2} \cdot \frac{S_2}{K_S + S_2 + \frac{S_2}{K_i}} \tag{4}$$

where μ_{max2} is the maximum bacterial growth rate regardless of inhibition, K_s is the Michaelis–Menten constant or average saturation coefficient and K_i is the inhibition coefficient due to the substrate.

2.4. System of equations

The system of ordinary differential equations related to the biomass dynamics of the substrate is shown below.

$$\frac{dX_1(t)}{dt} = (\mu_1 - D - K_{d1}) X_1 \tag{5}$$

$$\frac{dS_1(t)}{dt} = D(S_{in_1} - S_1) - \alpha_1 \mu_1 X_1 \tag{6}$$

$$\frac{dX_2(t)}{dt} = \left(\mu_2 - D - K_{d2}\right)X_2 \tag{7}$$

$$\frac{dS_2(t)}{dt} = D\left(S_{in_2} - S_2\right) - \alpha_4\mu_1 X_1 - \alpha_7\mu_2 X_2 \tag{8}$$

2.5. AM2 steady state model

A system is considered to reach steady state when its characteristics do not vary over time [2,9,10]. Knowing this and taking into account the processes and variables considered in the model, in order to obtain the steady state of the system for biomasses and substrates it is established that:

$$\begin{cases} \left(\mu_1 - D - K_{d_1}\right)X_{re_1} = 0 \\ D\left(S_{in_1} - S_{re_1}\right) - \alpha_1\mu_1 X_{re_1} = 0 \end{cases} \tag{9}$$

The equations for the digestion of sugars being (S_1),

$$\begin{cases} \left(\mu_2 - D - K_{d_2}\right)X_{re_2} = 0 \\ D\left(S_{in_2} - S_{re_2}\right) - \alpha_4\mu_1 X_1 - \alpha_7\mu_2 X_2 = 0 \end{cases} \tag{10}$$

And being the corresponding equations for methanogenesis of acetic acid (S_2).

Assuming that the biomass concentrations are non-zero and from the above equations, it is considered that:

$$\begin{cases} \left(\mu_1 - D - K_{d_1}\right) = 0 \\ \left(\mu_2 - D - K_{d_2}\right) = 0 \end{cases} \tag{11}$$

Substituting in each of the expressions the corresponding value of its own kinetics (2), (4) becomes as follows:

$$\begin{cases} \mu_{max1} \cdot \dfrac{S_1}{K_{s_1} + S_1} - D - K_{d_1} = 0 \\ \mu_{max2} \cdot \dfrac{S_2}{K_{s_2} + S_2 + \dfrac{S^2}{K_i}} - D - K_{d_2} = 0 \end{cases} \tag{12}$$

By subtracting the substrate concentration from each of the equations, the steady-state values are obtained for each of them.

Eq. (13) for sugars and Eq. (14) for acetic acids:

$$S_{re_2} = \frac{\left(D + K_{d_1}\right)\cdot K_{s_1}}{\mu_{max1} - D - K_{d_1}} \tag{13}$$

$$S_{re_2} = \frac{-\left(1 - \dfrac{\mu_{max2}}{D + K_{d_2}}\right)K_i \pm \sqrt{\left(1 - \dfrac{\mu_{max2}}{D + K_{d_2}}\right)^2 K_i^2 - 4K_{s_2}K_i}}{2} \tag{14}$$

By subtracting the value of X_{re1} and X_{re2} in the second expression (5) of the equations and substituting the values already calculated for each of the substrates, we obtain their respective steady-state values for each of the biomasses.

Eq. (15) for sugars and Eq. (16) for acetic acids:

$$X_{re_1} = \frac{D\left(S_{in_1} - S_{re_1}\right)\left(S_{re_1} + K_{s_1}\right)}{\alpha_1\mu_{max1}S_{re_1}} \tag{15}$$

$$X_{re_2} = \left(D\left(S_{in_2} - S_{re_2}\right) + \alpha_4\mu_{max1}\frac{S_{re_1}}{K_{s_1} + S_{re_1}}X_{re_1}\right)\left(\frac{S_{re_2}K_i + K_{s_2}K_i + S_{re_2}^2}{\alpha_7\mu_{max2}S_{re_2}K_i}\right) \tag{16}$$

3. Transitional regime

When there is a change in the variables of the system, we say that the process is in a transient regime [9,10,13]. When the conditions of an element change, the steady state is lost, and after a succession of changes it returns to equilibrium. The interval between the two steady states is called the transient regime.

As previously explained, a reactor can be considered as a continuous load, where the load is introduced in a constant way, or discontinuous, where the load is introduced in batches, an incoming flow $\hat{Q}$, which is equivalent to the volume of load V_1 between the load time T, is introduced. In this section, in addition to seeing what the system is like in a transient state, the difference between a batch and a continuous load [10] will be observed.

3.1. Batch loading

Batch loading involves the introduction of a given volume V_1, with an organic load, in a very short time [10]. The volume V_1, of the load, each time it is introduced, displaces an amount of volume equal to V_1, being the total volume of the digester V_T, and the volume not displaced is V_2, so we have:

$$V_T = V_1 + V_2 \tag{17}$$

Once the loading is done, the volume of liquid with the organic matter is assumed to be perfectly mixed at the same time of loading. As a consequence of the above, the dilution becomes the following expression:

$$D = \frac{\hat{Q}}{V_1 + V_2} = \frac{\dfrac{V_1}{T}}{V_T} \tag{18}$$

where $\hat{Q}$ is the inlet flow rate, T the loading time, V_1 the loading volume, V_T the total digester volume. To adapt the model to the batch inlet the following is considered.

$$\left.\begin{array}{l} \dfrac{dX}{dt} = \left(\mu - k_d\right)X \\ \dfrac{dS}{dt} = -\alpha\mu X \end{array}\right\} \leftrightarrow t \neq nT \tag{19}$$

When charging is not carried out:

$$\left.\begin{aligned}\Delta S &= \frac{V_1}{V_T}\left(S_{\text{in}} - S^*\left(nT\right)\right)\\ \Delta X &= \frac{V_1}{V_T}\left(X_{\text{in}} - X^*\left(nT\right)\right)\end{aligned}\right\} \leftrightarrow t = nT \tag{20}$$

When loading is performed, $S^*(nT)$ being the concentration of the substrate just before loading. The concentration is $S(nT)$ after charging and mixing.

$$S\left(nT\right) = \frac{S_{\text{in}}V_1 + S^*\left(nT\right)V_2}{V_T} \tag{21}$$

For all the present species considered in this final degree project, the mixture is as follows:

$$S_1 = \frac{S_{\text{in}_1}V_1 + S_1^*V_2}{V_T} \tag{22}$$

$$X_1 = \frac{X_{\text{in}_1}V_1 + X_1^*V_2}{V_T} \tag{23}$$

$$S_2 = \frac{S_{\text{in}_2}V_1 + S_2^*V_2}{V_T} \tag{24}$$

$$X_2 = \frac{X_{\text{in}_2}V_1 + X_2^*V_2}{V_T} \tag{25}$$

3.2. Batch system of equations

The system of batch equations when no loading (26) and when loading (27) with biomass and substrate dynamics is performed is as shown below.

$$\left.\begin{aligned}\frac{dX_1\left(t\right)}{dt} &= \left(\mu_1 - K_{d_1}\right)X_1\\ \frac{dS_1\left(t\right)}{dt} &= -\alpha_1\mu_1X_1\\ \frac{dX_2\left(t\right)}{dt} &= \left(\mu_2 - K_{d_2}\right)X_2\\ \frac{dS_2\left(t\right)}{dt} &= \alpha_4\mu_1X_1 - \alpha_7\mu_2X_2\end{aligned}\right\} \leftrightarrow t \neq nT \tag{26}$$

$$\left.\begin{aligned}X_1 &= \frac{V_1}{V_T}\left(X_{\text{in}_1} - X_1^*\left(nT\right)\right)\\ S_1 &= \frac{V_1}{V_T}\left(S_{\text{in}_1} - S_1^*\left(nT\right)\right)\\ X_2 &= \frac{V_1}{V_T}\left(X_{\text{in}_2} - X_2^*\left(nT\right)\right)\\ S_2 &= \frac{V_1}{V_T}\left(S_{\text{in}_2} - S_2^*\left(nT\right)\right)\end{aligned}\right\} \leftrightarrow t = nT \tag{27}$$

3.3. Numerical method for a batch system

Since the system of equations shows non-linear relationships in the state variables, it is necessary to apply a numerical approximation of the problem in order to solve it. The latter involves applying the procedures typical of initial value problems. In this work we propose to use a method called predictor–corrector, which is based on the use of an explicit solution as the initial predictor solution, and then from this, an implicit solution will be used iteratively until the solution converges, with a tolerance [8,10]. The solutions used are: for the predictor, the simplest Euler form, in its explicit form, as shown below:

$$\frac{dy\left(t\right)}{dt} = f\left(t, y\left(t\right)\right), \qquad y\left(t_0\right) = y_0 \tag{28}$$

$$y_{n+1} = y_n + hf\left(t_n, y_n\right) \qquad t_0 = t_0 + nh \tag{29}$$

And for the corrector the implicit Crank–Nicolson solution, or also equivalent to a trapezoidal solution. This solution is shown below:

$$\frac{dy\left(t\right)}{dt} = f\left(t, y\left(t\right)\right), \qquad y\left(t_0\right) = y_0 \tag{30}$$

$$y_{n+1} = y_n + \frac{h}{2}\left[f\left(t_n, y_n\right) + f\left(t_{n+1}, y_{n+1}\right)\right], \qquad t_n = t_0 + nh \tag{31}$$

Unifying the two solutions in the prediction–correction process leaves:

$$y_{n+1}^{(P} = y_n + hf\left(t_n, y_n\right) \rightarrow \qquad \text{Prediction} \tag{32}$$

$$y_{n+1}^{(C_o} = y_n + \frac{h}{2}\left[f\left(t_n, y_n\right) + f\left(t_{n+1}, y_{n+1}^{(P}\right)\right] \rightarrow \qquad \text{Start up} \tag{33}$$

$$y_{n+1}^{(C_{k+1}} = y_n + \frac{h}{2}\left[f\left(t_n, y_n\right) + f\left(t_{n+1}, y_{n+1}^{(C_k}\right)\right] \rightarrow \qquad \text{Correction} \quad \left|y_{n+1}^{(C_{k+1}} - y_{n+1}^{(C_k}\right| < \in \tag{34}$$

As indicated, this iterative process will continue until the convergence specifications are met.

As an example, the proposed system of equations for the sugar degrading biomass is shown in the following example, explicit (35), implicit (36) and Crank–Nicolson (37).

$$\frac{X_{1_n} - X_{1_{n-1}}}{\Delta t} = \left(\mu_{\max 1}\frac{S_{1_{n-1}}}{K_{s_1} + S_{1_{n-1}}} - K_{d_1}\right)\cdot X_{1_{n-1}} \tag{35}$$

$$\frac{X_{1_n} - X_{1_{n-1}}}{\Delta t} = \left(\mu_{\max 1}\frac{S_{1_n}}{K_{s_1} + S_{1_n}} - K_{d_1}\right)\cdot X_{1_n} \tag{36}$$

$$\frac{X_{1_n} - X_{1_{n-1}}}{\Delta t} = \frac{\mu_{\max 1}}{2}\left[\left(\frac{S_{1_{n-1}}X_{1_{n-1}}}{K_{s_1} + S_{1_{n-1}}} - K_{d_1}\right) + \left(\frac{S_{1_n}X_{1_n}}{K_{s_1} + S_{1_n}} - K_{d_1}\right)\right] \tag{37}$$

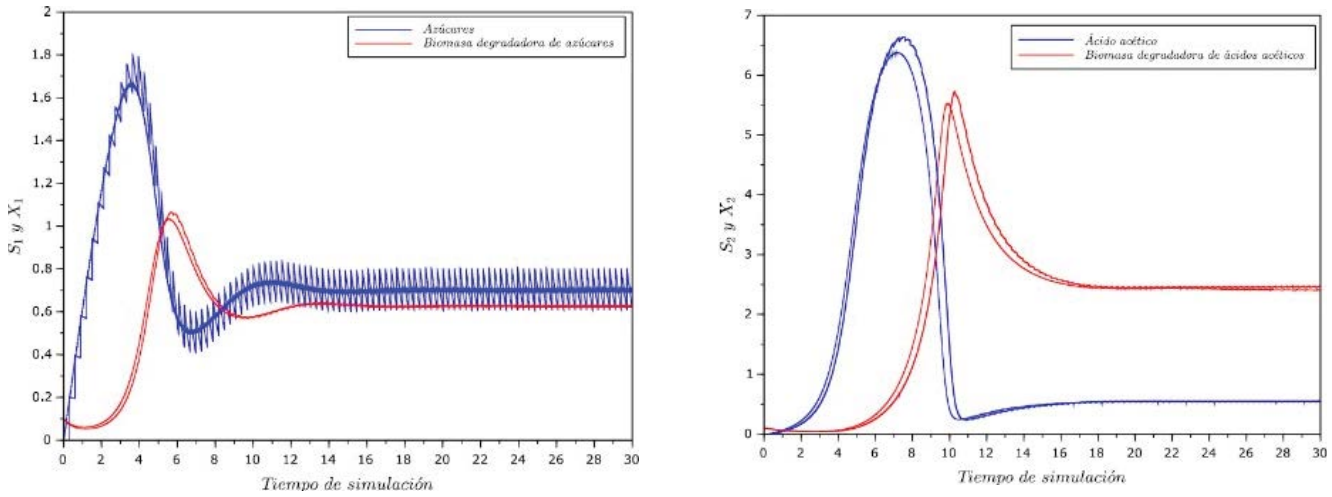

Fig. 1. Transient state of sugars at different loadings and the transient state of acetic acids at different loadings.

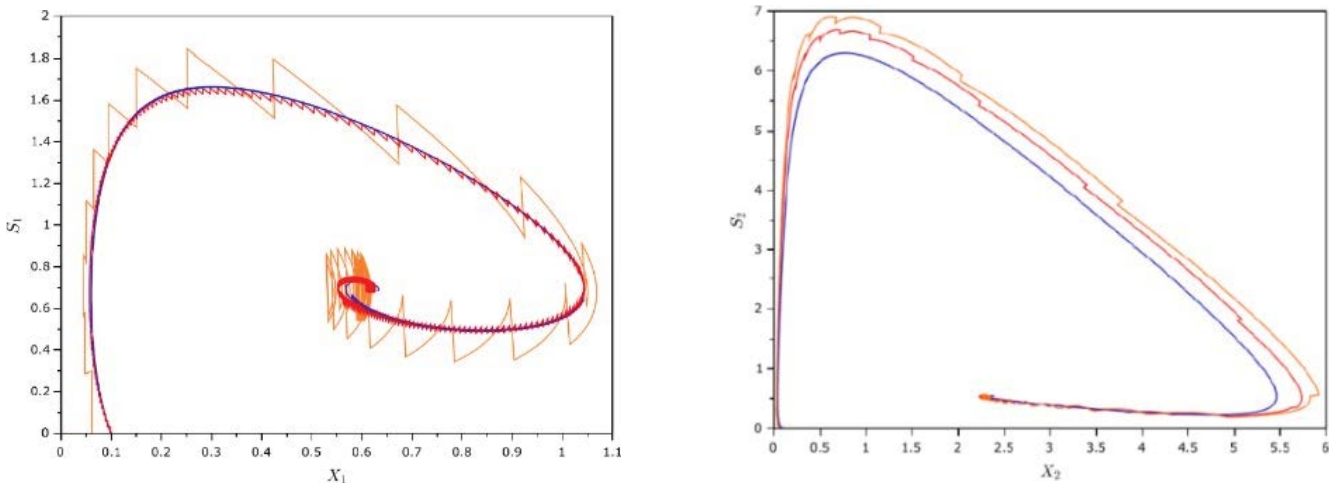

Fig. 2. Phase plane of sugars and acetic acid in transient state at different loadings.

4. Results

This section shows the results obtained from the simulation of the behaviour of X_1 and X_2 and substrates, under a continuous and a discontinuous load in a transient regime, depending on the simulation time. For this simulation, it is necessary to vary the inlet flow rate and the time between loading and loading. For this purpose, a continuous load and a discontinuous load have been considered, where V_1 is 0.01 L, always having a total volume of 10 L. Moreover, the working conditions are the same in both simulations where the inlet concentration of sugars is 20 and at a dilution of 30.

Fig. 1 shows how the biomass and substrate concentrations are affected by the type of load, in terms of substrate it can be seen that the peaks are produced by the introduction of the load and the decrease by the consumption of this in the reactor, producing a small oscillation in the number of sugar degrading bacteria. This effect is also seen in the acetic acid degrading bacteria causing a shift in production.

Fig. 2 shows the same way in the phase plane, but at three different loads, the blue, continuous load, the red, batch load explained above and the orange, batch load, where V_1 is 0.015 L under the same conditions. By varying the loads from continuous to batch loads, the process is affected, but leads to the same steady state. However, it must be taken into account that in order to avoid bacterial depletion, as the time between loading and loading increases, the loading volume has to be increased.

5. Conclusions

In this work, the proposed model has proved to be an effective tool for the estimation of the anaerobic digestion process and for learning the continuous and discontinuous dynamics of anaerobic digesters. Moreover, the open-source mathematical calculation program SCILAB is a suitable tool to carry out a mathematical modelling project of this type, since it is a very flexible platform that allows the user to simulate the dynamic conditions that occur during the anaerobic digestion process, being, on the other hand, easy to apply

in training activities for students of the University Degrees and Masters with competences in the area of environmental technology.

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