A Formal Modeling Framework for Anaerobic Degestion Systems

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Abstract—The complexity of modeling the anaerobic digestion process meets the difficulty to describe and analyze them mathematically. In this paper, a simplified mathematical model for anaerobic digestion process of organic matter, in a continuous stirred tank reactor is proposed. With the aim of upgrading the produced biogas and integrate biogas plants in a virtual power plant, new control inputs reflecting addition of stimulating substrates (acetate and bicarbonate) are added. Based on two step (acedogenesis-methanogenesis) mass balance non linear model, a step-by-step model parameter's identification procedure is presented in the first step, then in the second step, the yield coefficients and the microbial growth rates are estimated when the later is assumed to be unknown a priori.

Keywords–Anaerobic Digestion; Non-linear Models; Non-Linear Identification; Virtual Power Plants

I. INTRODUCTION

Anaerobic digestion process (AD) is a promising method for solving both energy and ecological problems. It consists on degrading organic matter (proteins, fats and carbohydrates) through a series of chemical and physicochemical reactions mediated, by anaerobic bacteria, to become it in biogas. The later is a potential energy which could be used to stabilize the power network. Despite the numerous advantages of the AD process, it is still bad responded in industry due to its instability characteristic, high sensor costs and difficult measurement procedures. Therefore, a mathematical modeling and software sensors are a great alternative to improve the process.

Modeling the AD process has been widely investigated in the last decades, we can find more than 70 models in the literature [1], and [2]. However, most of the existing models focus on the comprehension of the biological process, as is the case of $ADM1$ for instance [3], and result in complex models unsuitable for control. Similarly much of those built for control purpose, allow it only by acting on the waste feed rate to the digester [5], [10]. This means that the constraints on the waste storage and the plant infrastructure were not considered, whereas this is far away for being true in the real life. However, some of waste treatment plants are constrained to treat a precise quantity of waste per day.

Therefore, to overcome the mentioned constraint, we propose a simplified model allowing the transfer of the experimental results from a laboratory scale to a real life operation scale. This is done, by the addition of two new control inputs reflecting the addition of a stimulating substrates in order to upgrade the produced biogas, while optimizing the system.

The first suggested control input is the acetate addition which is commonly used to increase the biogas quantity. However, the acetate addition causes pH breakdown especially in low buffering capacity reactors, hence it is always accompanied by pH increase (increase till $pH = 8.5$ [9]) of the inlet waste. Often, the way pH is increased is not optimal for the process since it does not take into account dynamics of inorganic carbon and alkalinity inside the reactor. Therefore, we added the second control input to control the bicarbonate addition in function of the reactor state.

The paper is organized as follows. In the next section II, we describe the proposed six order mass balance non-linear model followed by our proposed step-by-step identification procedure that is discussed in Section III. In Section IV, we propose an adaptive estimation of the yield coefficients and the specific reaction rates when no a priori knowledge about the biomass growth rates is available. Finally, we conclude the paper in Section V.
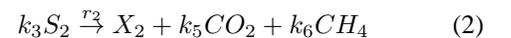
II. MODEL DESCRIPTION

It is well known that AD is a delicate process involving several microbial species [2], [3], and [7], and usually the model complexity is directly linked to the considered involved bacteria. Therefore, a two-step process (acedogenesis and methanogenesis) has often been reported in the literature to be suitable for the control purpose [5],[6], [7], and [10]. Hence, similarly the proposed model consider the following limiting steps:

1) Acidogenesis with reaction rate $r_1 = \mu_1 X_1$

$$k_1 S_1 \xrightarrow{r_1} X_1 + k_2 S_2 + k_4 CO_2 \qquad (1)$$
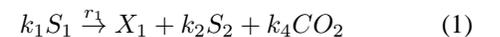
2) Methanogenesis with reaction rate $r_2 = \mu_2 X_2$

$$k_3 S_2 \xrightarrow{r_2} X_2 + k_5 CO_2 + k_6 CH_4 \qquad (2)$$

where in the first step, acedogenic bacteria (X_1) consume the organic substrate (S_1) and produce volatile fatty acids (VFA) and CO_2. In the second step, the produced VFA (S_2) are consumed by methanogenic bacteria (X_2) for growth and produce CO_2 and methane.

To model the considered limiting steps (1) and (2) while including the new control inputs, we assume that the reactor is perfectly stirred (thus biomass is uniformly distributed in the reactor), pH and temperature (T) range between 6 to 8 and 35 to 38^0C, respectively, and finally VFA (S_2) behave like pure acetate.

A. Model Equations

We denote the state vector by $\xi = [X_1, S_1, X_2, S_2, C, Z]^T$, where ^{T} represents the transposed operator. The state vector is described by the following equations.

$$
\begin{aligned}
\dot{X}_1 &= (\mu_1(\xi) - D)X_1 \\
\dot{S}_1 &= -k_1\mu_1(\xi)X_1 - DS_1 + D_1S_{1in} \\
\dot{X}_2 &= (\mu_2(\xi) - D)X_2 \\
\dot{S}_2 &= k_2\mu_1(\xi)X_1 - k_3\mu_2(\xi)X_2 - DS_2 \\
&\quad + D_1S_{2in} + D_2S_0' \\
\dot{C} &= k_4\mu_1(\xi)X_1 + k_5\mu_2(\xi)X_2 - DC \\
&\quad + D_1C_{in} + D_3C_0' - Q_c \\
\dot{Z} &= -DZ + D_1Z_{in}
\end{aligned}
\quad (3)
$$

each one of the elements of Eq. (3) reflects the mass balance of its corresponding state. Here, $X_i(g.L^{-1})$, $S_1(g.L^{-1})$, S_2 $(mmole.L^{-1})$, and $\mu_i(\xi)(day^{-1})$ are the bacteria concentration, the associated substrate concentrations, and the bacteria growth rates. Both rates are given by:

$$
\begin{cases}
\mu_1(S_1) = \mu_{1max}\frac{S_1}{S_1+k_{s1}} & (Monod) \\
\\
\mu_2(S_2) = \mu_{2max}\frac{S_2}{S_2+k_{s2}+\frac{S_2^2}{k_{I2}}} & (Haldane)
\end{cases}
\quad (4)
$$

With the undertaken pH and the temperature (T) assumptions, the total dissolved inorganic carbon concentration C $(mmole.L^{-1})$ is the sum of bicarbonate (Bic) and the dissolved CO_2 concentrations. Similarly, the alkalinity concentration Z $(mmole.L^{-1})$ is the sum of bicarbonate (Bic) and dissociated acids S_2 $(mmole.L^{-1})$ mainly acetate. They are given by:

$$
\begin{cases}
Z = Bic + S_2 \\
C = CO_2 + Bic \\
p_H(\xi) = -\log_{10}(K_b\frac{CO_2}{Bic})
\end{cases}
\quad (5)
$$

The gaseous flow rates Q_c and Q_M of CO_2 and CH_4, respectively, are given as proposed in the $AM2G$ model [4].

$$
\begin{cases}
Q_c(\xi) = \frac{RT\gamma CO_2}{P_T+RT\gamma(K_HP_T-CO_2)}Q_M \\
\\
Q_M(\xi) = k_6\mu_2(\xi)X_2
\end{cases}
\quad (6)
$$

where γ is the dimensionless parameter introduced by Hess [4] in order to reduce the expression complexity between the dissolved and the gaseous CO_2.

K_i are the yield coefficients defined in (I) and (II) with other parameters. ξ_{in} are inlet waste concentrations fed to the digester with dilution rate D_1, D_2 is the dilution rate for the first added stimulate substrate (acetate) with concentration S_0', and D_3 is the dilution rate for the second added stimulate substrate (sodium bicarbonate) with concentration C_0'. D is the total dilution rate ($D = D_1 + D_2 + D_3$).

B. Model Steady States

It is well known that biological processes exhibit multiple equilibrium states and the AD process takes part too. If we do not consider the washout of bacteria steady state ($X_1 = 0$ or $X_2 = 0$), the steady states of the state model of the Eq. (3) are given by:

$$
\begin{cases}
\mu_1(S_1) = D & (7a) \\
\\
\mu_2(S_2) = D & (7b) \\
\\
S_1^* = k_{s1}\dfrac{D}{\mu_{1max} - D} & (7c) \\
\\
\dfrac{S_2^{*2}}{k_{I2}} + S^*(1 - \dfrac{\mu_{2max}}{D}) + k_{s2} = 0 & (7d) \\
\\
X_1^* = \dfrac{1}{k_1}\left(\dfrac{D_1}{D}S_{1in} - S_1^*\right) & (7e) \\
\\
X_2^* = \dfrac{1}{k_3}\left(\left(\dfrac{D_1}{D}S_{2in} - S_2^*\right) + \dfrac{k_2}{k_1}\left(\dfrac{D_1}{D}S_{1in} - S_1^*\right)\right) \\
\qquad + \dfrac{D_2}{k_3D}S_0' & (7f) \\
\\
Z^* = \dfrac{D_1}{D}Z_{in} & (7g) \\
\\
C^* = \left(\dfrac{k_4}{k_1} + \dfrac{k_5k_2}{k_3k_1}\right)\left(\dfrac{D_1}{D}S_{1in} - S_1^*\right) \\
\qquad + \dfrac{k_5}{k_3}\left(\dfrac{D_1}{D}S_{2in} - S_2^*\right) \\
\qquad + \dfrac{1}{D}\left(\dfrac{k_5}{k_3}S_0' + D_1C_{in} + D_3C_0' - Q_c(\xi^*)\right) & (7h) \\
\\
Q_M(\xi^*) = \dfrac{k_6}{k_3}((D_1S_{2in} - D.S_2^*)) + \\
\qquad \dfrac{k_2}{k_1}((\dfrac{D_1}{D}S_{1in} - D.S_1^*)) \\
\qquad + \dfrac{k_6.D_2}{k_3}S_0' & (7i)
\end{cases}
$$

Solutions of Eq. (7d) are the possible steady states for acetate (S_2), where the largest one corresponds to methanogenesis inhibition phase (a detailed study of the corresponding equilibrium can be found in [4]).

Equilibrium of the dissolved inorganic carbon (C) are obtained from Eqs (5), (6) and (7h). They are solutions of the following second degree equation:

$$
\begin{aligned}
0 = {}& D\beta C^{*2} \\
& - DC^*(P_T + \beta(K_HP_T + Z^* - S_2^* + k_4X_1^*) \\
& - DC^*(+k_5X_2^* + k_6X_2^* + \tfrac{D_1}{D}C_{in} + \tfrac{D_3}{D}C_0') \\
& + D(P_T + \beta(K_HP_T + Z^* - S_2^*)(k_4X_1^* + k_5X_2^*) \\
& + D(k_6X_2^* + \tfrac{D_1}{D}C_{in} + \tfrac{D_3}{D}C_0')) \\
& + D\beta(Z^* - S_2^*)k_6X_2^*
\end{aligned}
\quad (8)
$$

with $\beta = RT\gamma$.

In order to analyze (8), we rewrite it in the standard form as:

$$0 = f(C^*) = aC^{*2} - bC^* + d \qquad (9)$$

where a, b and d are positive values.

By definition sum and product of this polynomial roots are positive, given by:

$$C_i^* = \frac{b + (-1)^i \sqrt{\Delta}}{2a} \qquad (10)$$

and evidently have positive real part.

To show that the roots (10) are real, we study the real function f.

It can be easily shown from (8) that $f(0) > 0$ and $\lim_{C \to +\infty} f(C) = +\infty$. Moreover, the retained root should verify the positivity of CO_2 flow rate ($Q_c^* > 0$) at the steady state. From (6), this condition is verified if:

$$C^* < \frac{P_T + \beta(K_H P_T + Z^* - S_2^*)}{\beta} = C_c$$

If, we calculate the polynomial (8) value for C_c, we find:

$$f(C_c) = -(P_T + \beta K_H P_T)k_6 X_2^* < 0 \qquad (11)$$

From (10), we know that the polynomial has two roots and it is of sign $-a$ in between. Hence, we deduce from (11) that $C_1^* < C_c < C_2^*$ and we conclude that C_1 is the only physically admissible root in the case of normal operating point.

III. PARAMETERS IDENTIFICATION

Since new inputs have been introduced in the model given by Eq. (3), it is mandatory to precise some of input's coefficients. Unfortunately, the not differentiability of parameters for such models is a well known issue. It has been reported in [13] [12] that different sets of coefficients can provide similar simulation results, and more, different coefficient values result for different particular organic matter [10], [11], [12]. Therefore a step-by-step identification procedure is often applied to solve this problem.

Hence, taking advantageous from the cascade structure of the model proposed in (3), we separate the parameters in different groups in order to identify them as independently as possible from each other. In the first step, we proceed as reported in [6] while estimating the parameters in steady state to force the model to correctly predict the equilibrium state to be reached by the system. In the second step, a calibration procedure based on non-linear optimization is to be performed.

While building the model, one should exploit as much as possible the available measurements and has to choose carefully the experiment conditions so as to cover as much as possible the range of the expecting operation situations.

Therefore, for the first step mean values of different steady states for $\overline{S_1}$, $\overline{S_2}$, $\overline{Z}$, $\overline{C}$, $\overline{pH}$, $\overline{Q_c}$ and $\overline{Q_M}$ are to be used.

The two separate considered groups of parameters are the kinetic parameters (k_{s1}, k_{s2}, k_{I2}, μ_{1max}, μ_{2max}) and the coefficient γ in the first group, while the yield coefficients in the second one.

A. Kinetic Parameters and γ Identification

From Eq. (7a) we obtain:

$$\frac{1}{D} = \frac{1}{\mu_{1max}} + \frac{k_{s1}}{\mu_{1max}} \frac{1}{\overline{S_1}} \qquad (12)$$

that can be used to estimate μ_{1max} and k_{s1} by a linear regression.

Similarly from Eq. (7b), we obtain the following relationship:

$$\frac{1}{D} = \frac{1}{\mu_{2max}} + \frac{k_{s2}}{\mu_{2max}} \frac{1}{\overline{S_2}} + \frac{1}{k_{I2}} \frac{1}{\mu_{2max}} \overline{S_2} \qquad (13)$$

which is used to estimate k_{I2}, k_{s2} and μ_{2max} by a linear regression too.

From Eqs. (5) and (6), we express the following relationship:

$$\frac{1}{\overline{Q_c}} = \frac{1}{\gamma} \frac{P_T}{RT(\overline{C} - \overline{Z} + \overline{S_2})} \frac{1}{\overline{Q_M}} + \left(\frac{K_H P_T - \overline{C} - \overline{Z} + \overline{S_2}}{\overline{C} - \overline{Z} + \overline{S_2}} \right) \frac{1}{\overline{Q_M}} \qquad (14)$$

from which a linear regression gives the value of the dimensionless parameter γ.

B. Yield Coefficients Identification

Using steady state equations given in Eqs. (6), (7h), and (7i), and the mean measurement values used previously, we can estimate the ratio of yield coefficients $\frac{k_6}{k_3}$, $\frac{k_2}{k_1}$, $\frac{k_4}{k_1}$ and $\frac{k_5}{k_3}$ by a linear regression applied to the following equations:

$$\overline{Q_M} = \frac{k_6}{k_3}((D_1 S_{2in} - D\overline{S_2}) + \frac{k_2}{k_1}(D_1 S_{1in} - D\overline{S_1})) + \frac{k_6}{k_3} D_2 S_0' \qquad (15)$$

$$\overline{Q_c} = \left(\frac{k_4}{k_1} + \frac{k_5 k_2}{k_3 k_1} \right) (D_1 S_{1in} - D\overline{S_1}) + \frac{k_5}{k_3}(D_1 S_{2in} - D\overline{S_2} + (\frac{k_5}{k_3} S_0' + D_3 C_0') + (D_1 C_{in} - D\overline{C}) \qquad (16)$$

So, the Eq. (16) can be rewritten using the methane flow rate measurement as follow:

$$\overline{Q_c} = \frac{k_2}{k_1}(D_1 S_1 in - D\overline{S_1}) + \frac{k_5}{k_6}\overline{Q_M} + (D_1 C_{in} - D\overline{C}) \qquad (17)$$

As it can be seen from Eqs. (15), (16) and (17), only the ratio of yield coefficients can be estimated from the used measurements. This issue was widely discussed in literature (see [6] and [10]). In fact, yield coefficients can be estimated only if acidogenic and methanogenic bacteria measurements ($\overline{X_1}$ and $\overline{X_2}$ respectively) are available.

Hence, we need to estimate the separate yield coefficients if we want to obtain the biomass concentration in the reactor. However, measuring biomass concentrations is unsuitable due to its complexity. Bernard et al. [6] proposed to use the volatile suspended solids (VSS) measurement as a rough approximation for the total biomass concentration $X_1 + X_2$. Then, estimate each concentration separately using the ratio $v = 0.2$ of acidogenic and methanogenic bacteria taken from [14]. Hence, by using the equilibrium steady state (7e), we have:

$$v = \frac{\overline{X_1}}{\overline{X_1} + \overline{X_2}} \approx \frac{1}{k1} \frac{\frac{D_1}{D}S_{1in} - S_1}{\overline{VSS}} \quad (18)$$

if v is assumed to be constant k_1 is estimates by:

$$k_1 = \frac{1}{v} \frac{\frac{d_1}{d}s_{1in} - s_1}{\overline{vss}} \quad (19)$$

Now, using Eqs. (7e) and (7f), we get:

$$v = \frac{k_3}{k_1} \times$$
$$\frac{\frac{D_1}{D}S_{1in} - S_1}{(\frac{k_3}{k_1} + \frac{k_2}{k_1})(\frac{D_1}{D}S_{1in} - S_1) + \frac{D_2}{D}S_{2in} - S_2 + \frac{D_2}{D}S_0'} \quad (20)$$

thus k_3, can be estimated as follows:

$$k_3 = k_1 \left(\frac{v}{1-v} \right) \left(\frac{k_2}{k_1} + \frac{\frac{D_2}{D}S_{2in} - S_2 + \frac{D_2}{D}S_0'}{\frac{D_1}{D}S_{1in} - S_1} \right) \quad (21)$$

Finally, by using the yield coefficient ratios identified before, we can deduce all the yield coefficients estimates.

C. Calibration

Till now the yield coefficients for the steady state were estimated. This was possible by taking some assumptions like the constancy of the acidogenic and methanogenic ratio v, and the correlation between VSS measurement and the biomass concentration in the reactor and, last but not least, the certainty of measurements at steady state. Therefore, to enable the model to predict as correct as possible the process behavior in both steady and transient states, we propose to calibrate the yield coefficients using online data measurements.

Usually, very restrictive information about the process can be obtained and only acetate S_2, alkalinity Z, and gaseous flow rates are measured for known inputs (often uncertain input concentrations). Therefore, we assume that S_2, Z Q_c and Q_M are measured online to perform the nonlinear identification depicted in Fig. 1. where the criteriom J to minimize is:

$$J = \min_P \sum [L_1(S_{2mes} - S_{2mdl})^2 + L_2(Q_{Mmes} - Q_{Mmdl})^2 + L_3(Q_{Cmes} - Q_{Cmdl})^2 + L_4(Z_{mes} - Z_{mdl})^2] \quad (22)$$

with L_i are weight coefficients, and P a vector containing the parameters to be estimated.

Many optimization tools for non-linear identification with generated data from known models can be used to find the desired parameters. At this step, we use the previously found yield coefficients at steady state to initialize the non linear estimation algorithm and hence, we avoid biased estimates which usually occur when the algorithm is bad initialized. Actually, a simple iterative parameter estimation based on sensitivity analysis and non linear optimization methods has been proposed in [13]. We, suggest to use while initializing it by the previously found yield coefficients.

IV. ADAPTIVE PARAMETERS ESTIMATION

In this section, we describe briefly how to estimate simultaneously the yield coefficients and the growth rates when no a priori knowledge of the later analytic expression is available. This means that the operator have no knowledge about the factors which can influence the biomass growth. For seek of brevity, we describe the steps of the method without going in the mathematical details. First, lets rewrite the state model (3) in a matricial form:

$$\begin{bmatrix} \dot{X_1} \\ \dot{S_1} \\ \dot{X_2} \\ \dot{S_2} \\ \dot{C} \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -k_1 & 0 \\ 0 & 1 \\ k_2 & -k_3 \\ k_4 & k_5 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mu_1 X_1 \\ \mu_2 X_2 \end{bmatrix} - D \begin{bmatrix} X_1 \\ S_1 \\ X_2 \\ S_2 \\ C \\ Z \end{bmatrix}$$
$$+ \begin{bmatrix} 0 \\ D_1 S_{1in} \\ 0 \\ D_1 S_{2in} + D_2 S_0' \\ D_1 C_{1in} + D_3 C_0' \\ D_1 Z_{in} \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ Q_c \\ 0 \end{bmatrix} \quad (23)$$

The general form of (23) is as follows:

$$\xi = K\phi(\xi) - D\xi + F - Q \quad (24)$$

Now, we split the state vector to tow sub-state vectors: ξ_1 contains the measurable states, and ξ_2 contains the remained not measurable states:

$$\xi_1 = K_1\phi(\xi) - D\xi_1 + F_1 - Q_1$$
$$\xi_2 = K_2\phi(\xi) - D\xi_2 + F_2 - Q_2 \quad (25)$$

Then, we introduce an auxiliary state $\zeta = A_0\xi_a + \xi_b$, where ξ_a and ξ_b are a nice partition allowing suppression of the unknown parameters from the dynamic of ζ, hence $A_0 = -K_2 K_1^{-1}$. Applying this model partition, widely discussed in [10], to the model (23) for $\xi_a = [X_1, X_2]^T$ and $\xi_b = [S_1, S_2, C, Z]^T$, we get the following relationship:

$$\zeta = \begin{bmatrix} k_1 & 0 \\ -k_2 & k_3 \\ -k_4 & -k_5 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + \begin{bmatrix} S_1 \\ S_2 \\ C \\ Z \end{bmatrix} \quad (26)$$
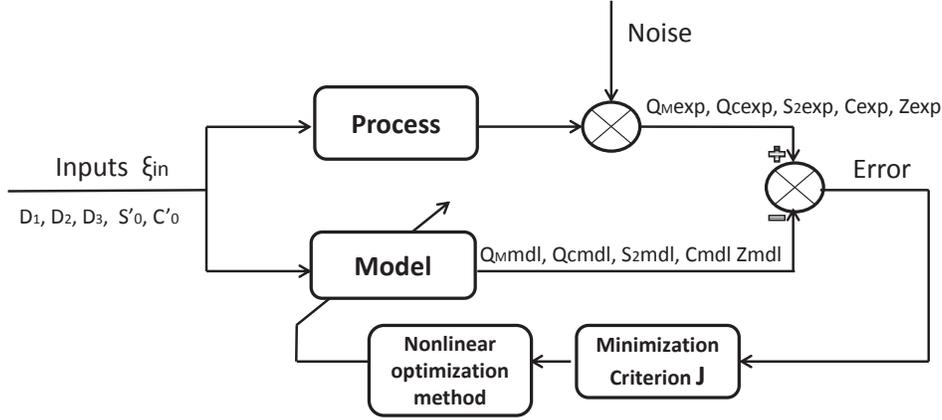
Figure 1. Non-Linear Identification Scheme.

and thus, the dynamic of ζ is given by:

$$\begin{bmatrix} \dot{\zeta_1} \\ \dot{\zeta_2} \\ \dot{\zeta_3} \\ \dot{\zeta_4} \end{bmatrix} = -D \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \end{bmatrix} \\ + \begin{bmatrix} D_1 S_{1in} \\ D_1 S_{2in} + D_2 S_0' \\ D_1 C_{1in} + D_3 C_0' - Q_c \\ D_1 Z_{in} \end{bmatrix} \quad (27)$$

Actually, now we can proceed for the yield and growth rates estimations using the new system containing the auxiliary state ζ and the measured state ξ_1 as described below. But, before proceeding with that we rewrite the product $\mu_i X_i$ as the product of the specific reaction α_i and the responsible components involved in the chemical reaction [10], thus we have:

$$\begin{aligned} \mu_1 X_1 &= \alpha_1 S_1 X_1 \\ \mu_2 X_2 &= \alpha_2 S_2 X_2 \end{aligned} \quad (28)$$

It has been already proved in the previous sections that yield coefficients can be estimated only if the biomass concentrations are measured. Hence, we assumed that $\xi_1 = [X_1, X_2, C]^T$ where using (28) its dynamic is given by:

$$\begin{bmatrix} \dot{X_1} \\ \dot{X_2} \\ \dot{C} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ k_4 & k_5 \end{bmatrix} \begin{bmatrix} \alpha_1 S_1 X_1 \\ \alpha_2 S_2 X_2 \end{bmatrix} - D \begin{bmatrix} X_1 \\ X_2 \\ C \end{bmatrix} \\ + \begin{bmatrix} 0 \\ 0 \\ D_1 C_{1in} + D_3 C_0' \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ Q_c \end{bmatrix} \quad (29)$$

Hence, the matrices A_1 and A_2 are the following:

$$A_1 = \begin{bmatrix} k_1 & 0 & 0 \\ -k_2 & -k_3 & 0 \\ -k_2 & k_5 & 1 \\ 0 & 0 & 0 \end{bmatrix}, A_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad (30)$$

Now the new state model to be processed contains ζ and ξ_1 described by (26) and (29), respectively.

In order to estimate the unknown yield coefficients and the specific reaction rates, we separate the known measurements from the unknown parameters. Therefore, the missed measurements are expressed in function of ξ_1 and ζ. Hence, the dynamic expression of ξ_1 is given as follows:

$$\xi_1 = \Psi(\xi_1, \zeta)\theta - D\xi_1 + F_1 - Q_1 \quad (31)$$

with $\Psi(\xi_1, \zeta)$ is given by (32), $\theta = [\alpha_1, k_1\alpha_1, \alpha_2, k_2\alpha_2, k_3\alpha_2, k_4\alpha_1, k_1k_4\alpha_1, k_5\alpha_2, k_2k_5\alpha_2, k_3k_5\alpha_2]^T$, $F_1 = [0, 0, D_1 C_{in} + D_3 + C_0']^T$ and finally $Q_1 = [0, 0, Q_c]^T$.

On the grounds of the previous transformations and definitions the vector θ (hence the unknown parameters) can be estimated using an observer based estimator like the following:

$$\begin{aligned} \dot{\hat{\zeta}} &= -D\hat{\zeta} + F_b - Q_b \\ \dot{\hat{\xi}}_1 &= \Psi(\xi_1, \hat{\zeta})\hat{\theta} - D\xi_1 + F_1 - Q_1 - \Omega(\xi_1 - \hat{\xi}_1) \\ \dot{\hat{\theta}} &= \Psi(\xi_1, \hat{\zeta})\Gamma(\xi_1 - \hat{\xi}_1) \end{aligned} \quad (33)$$

where Ω and Γ are design parameters, to be fixed by the designer so that the states given by the estimated parameters fit well the experiments data.

V. Conclusion

In order to facilitate the modeling aspect to control efficiently the anaerobic digestion process, we proposed a mathematical (formal) framework that describes how new stimulating substrates (acetate and bicarbonate) can be added to this process. This was motivated by the aim of controlling the quantity and the quality of the produced biogas from treatment plants in order to integrate them in a virtual power plant. To identify the model parameters, we proposed a step-by-step identification procedure based on two steps (acedogenesis-methanogenesis) mass balance

$$\phi = \begin{bmatrix} X_1\zeta_1 & X_1^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & X_2\zeta_2 & X_1X_2 & -X_2^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & X_1\zeta_1 & -X_1^2 & X_2\zeta_2 & X_1X_2 & -X_2^2 \end{bmatrix} \quad (32)$$

non linear model. Further, we described an online adaptive algorithm for yield coefficients and specific reaction rates estimation when no knowledge about the factors influencing the biomass behavior is available.

The research that we have initiated in this paper sets the fundamentals for further fully automatic modelling and analysis of biogas systems. First, we intend to validate our model on more realistic parameter. Then, we will propose new strategies of control to integrate the biogas plants in a virtual power plant to stabilize the power network.

ACKNOWLEDGMENT

VI. NOMENCLATURE

Acronyms	Definition
k_1	Yield for substrate degradation
k_2	Yield for VFA production
k_3	Yield for VFA consumption
k_4	Yield for CO_2 production
k_5	Yield for CO_2 production
k_6	Yield for Ch_4 production
μ_{1max}	Maximum acedogenic bacteria growth rate
μ_{2max}	Maximum methanogenic bacteria growth rate
k_{s1}	Half saturation constant associated with S_1
k_{s2}	Half saturation constant associated with S_2
K_{I2}	Inhibition constant associated with S_2
K_b	Acidity constant of bicarbonate
K_H	Henry s constant
R	Gas constant
P_T	Total preasure
T	Temperature
γ	dimonsionless parameter introduced by Hess [4]

TABLE I
NOMENCLATURE

Acronyms	Units
k_1	$g.g^{-1}$ of acidogenic bacteria
k_2	$mmole.g^{-1}$ of acidogenic bacteria
k_3	$mmole.g^{-1}$ of methanogenic bacteria
k_4	$mmole.g^{-1}$
k_5	$mmole.g^{-1}$
k_6	$mmole.g^{-1}$
μ_{1max}	day^{-1}
μ_{2max}	day^{-1}
k_{s1}	$g.l^{-1}$
k_{s2}	$mmol.l^{-1}$
K_{I2}	$mmol.l^{-1}$
K_H	$mmole.L^{-1}.atm^{-1}$
R	$L.atm.K^{-1}.mol^{mol}$
P_T	atm
T	Kelvin

TABLE II
NOMENCLATURE-CONTINUATION

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