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Highlights:

- 1. Robust nonlinear observer for on-line estimation of VFA in continuous Anaerobic Digesters.
- 2. Only the methane outflow rate is available for online measurement.
- 3. The proposed observer is able to the estimation of VFA in different operation conditions.
- 4. The observer convergence is analyzed by using Lyapunov stability techniques.

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# On-line estimation of VFA concentration in anaerobic digestion via methane outflow rate measurements

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#### Abstract

This paper deals with the design of a robust nonlinear observer as a software sensor to achieve the on-line estimation of the concentration of Volatile Fatty Acids (VFA) in a class of continuous Anaerobic Digesters (AD). Taking into account the limited availability of on-line sensors for AD process, in this contribution is assumed that only the methane outflow rate is available for online measurement. The estimation method is based on a modified version for a two-dimensional mathematical model of AD process. From the differential algebraic observability approach it is shown that the VFA concentration is detectable from the methane outflow rate measurements. The observer convergence is analyzed by using Lyapunov stability techniques. Numerical simulations illustrate the effectiveness of the proposed estimation method for a four-dimensional AD model with uncertainties associated with unmodeled dynamics and disturbances in the inflow composition.

*Key words:* Anaerobic Digestion; State observer; VFA estimation; Uncertain reaction systems; Software sensors.

#### 1. Introduction

The Anaerobic Digestion (AD) has gained considerable importance lately as a wastewater treatment technology to reduce organic matter in agro-food industrial wastes and municipal effluents. At the same time AD produces biogas, consisting firstly of methane ( $CH_4$ ) and carbon dioxide ( $CO_2$ ) and provides a versatile source of renewable energy, since the methane from biogas can be used for replacing the fossil fuels in both heat and power generation and as vehicle fuel (Weiland, 2010). From renewable power resource viewpoint, increasing the methane outflow rate is one of the key issues in the optimal operation of anaerobic processes (Kravaris & Savog-lidis, 2012; Lara-Cisneros et al., 2015; Stamatelatou et al., 1997). Nevertheless, its widespread application has been limited because of the difficulties involved in achieving stable operation of the AD process (Benyahia et al., 2012; Hess & Bernard, 2008; Schaum et al., 2015; Sbarciog et al., 2010, 2011). So that, the optimal operation of AD process is complicated to reach, mainly

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because of their highly nonlinear and unstable nature, inhibition by substrates or products and by the substantial unmodeled dynamics (Hess & Bernard, 2008; Sbarciog et al., 2010; Serhani et al., 2011; Shen et al., 2007). In fact, it is well known that the inhibition of the methanogenic bacteria growth by accumulation of Volatile Fatty Acids (VFA) induces the acidification of the system and leads to the process failure (Hess & Bernard, 2008; Sbarciog et al., 2010; Shen et al., 2007). Additionally, due to fluctuations in the inlet composition makes the optimal operation of the AD process very hard to keep in an open-loop configuration (Méndez-Acosta et al., 2008).

In this way, the implementation of innovative control schemes for optimal and robust stabilization of AD process requires advanced on-line measurement systems for a more adequate monitoring (Dochain, 2008; Lara-Cisneros et al., 2015). However, the existing monitoring equipment for critical variables of anaerobic processes such as organic acid concentrations and the main bacterial populations are too expensive and require extensive maintenance (Gaida et al., 2012). Only few variables as pH, temperature and gaseous outflow rate are available in a cost effective manner for on-line measurement. An interesting alternative is to take advantage of a mathematical model in conjunction with a limited set of available measurements that provides an estimate of the time evolution for the key process variables is the use of the so-called state observers (software sensors) (Luenberger, 1971; MohdAli et al., 2015). The design and application of state observers in bioprocesses has been an active area over the last decades (Bastin & Dochain, 1990; Dochain, 2003). Specifically for the AD process, in literature we can find different state estimation schemes from classical Kalman filters and adaptive observers schemes to asymptotic and interval observers (Bastin & Dochain , 1990; Bernard et al., 2000; Diop & Simeonov, 2009; Dochain, 2003, 2008; Gaida et al., 2012; Haugen et al., 2014; Kalchev et al., 2011; Rocha-Cózatl et al., 2015). The aim of most state observers proposed in literature is to provide the estimation for the key AD variables from the on-line measurement of the organic substrate concentration (expressed as chemical oxygen demand) or the total organic fatty acids concentrations (or both) (Rodríguez et al., 2015). However, in practice the biogas flow rate can be more easily measured on-line thats the organic substrates concentration or specific bacterial populations (Kalchev et al., 2011). In fact, today the advanced monitoring schemes are only possible by mean of spectroscopy-based instrumentation equipments (Madsen et al., 2011). The on-line estimation of the key variables in AD processes when only the biogas outflow rate is available for on-line measurement is an open issue in current literature. Nevertheless, only a few works can be found in open literature in regards to estimation schemes of AD from biogas outflow monitoring (Bernard et al., 2000; Carlos-Hernández et al., 2012; Diop & Simeonov, 2009; Haugen et al., 2014; Kalchev et al., 2011). In Bernard et al. (2000) an asymptotic observer has been proposed for estimation of COD and VFA from the on-line gaseous measurement. This kind of observers is based on a state transformation leading to a subsystem independent of the growth kinetics expressions. The main drawback of the asymptotic observers is that requires perfect knowledge of the yield coefficients (or a ratio of them), and may be very sensitive to unknown load disturbances (Diop & Simeonov, 2009). More recently, in Carlos-Hernández et al. (2012) is proposed a control strategy for bicarbonate regulation in AD process based in a fuzzy controller with a Takagi-Sugeno observer composed by 45 local observers. Also, in (Haugen et al., 2014; Kalchev et al., 2011) Kalman-type observers have been proposed for the estimation of key variables in AD process with only methane gas flow measurement. The main issue of the local observers approaches is their poor performance for operating condition far from of the designed conditions, mainly for strongly nonlinear and intrinsically unstable systems (Dochain, 2003).

In this contribution we propose a robust estimation method based on a nonlinear observer

composed by a linear plus sigmoid injection terms, with the aim of compute the time evolution of the VFA concentration in a class of AD process which uses only methane outflow rate measurement. In our contribution, the modified version for a two-dimensional mathematical model of AD process, that includes the dynamics for the methane outflow rate, is used to the observer design purpose. The detectability for VFA concentration is shown by applying the differential algebraic approach. The observer convergence is analyzed by using Lyapunov stability techniques. Numerical simulations illustrate the effectiveness of the proposed estimation method for a four-dimensional AD model with uncertainties associated with unmodeled dynamics and disturbances in the inflow composition. The rest of the paper is organized as follows: In Section 2 the AD mathematical model used in the observer design is presented, also the problem statement is presented and some issues related with the VFA detectability are discussed. Section 3 contains the design of the proposed observer scheme and its convergence properties are analyzed. Numerical experiments that illustrate the performance of the proposed estimation approach is shown in Section 4. Some concluding remarks are discussed in Section 5.

#### 2. Model description and problem statement

Let us consider a simple AD model proposed in Andrews (1968) that accounts for a single degradation stage of the soluble organic substrate (S) by the methanogenic biomass X.

$$k_t S \stackrel{\mu(\cdot)x}{\hookrightarrow} X + k_m CH_4$$

where  $k_t$  is the yield coefficient associated to substrate degradation and  $\mu(\cdot)$  stands for methanogenic bacterial growth rate. The corresponding mass-balance for a continuous anaerobic process it reads:

$$\dot{S} = u(S_f - S) - k_t \mu(\cdot) X \tag{1}$$

$$\dot{X} = \mu(\cdot)X - \alpha uX \tag{2}$$

where *u* is the dilution rate and  $\alpha$  is the fraction of bacterial not attached onto a support (i.e., being affected by the dilution rate in the digester). Because of the solubility of methane in the liquid phase is very low, the concentration of dissolved methane is neglected, and the produced methane is assumed to go directly out of the digester, with the outflow rate of methane gas  $Q_M$  proportional to the growth rate of the methanogenic biomass (see, Bernard et al. (2001))

$$Q_M = k_m \mu(\cdot) X \tag{3}$$

where  $k_m$  is the yield coefficient for the methane production. With respect to the specific growth rate for the methanogenic populations, in Bernard et al. (2001) it is assumed to be described by a nonmonotonic function of the substrate concentration, with the following properties:

**Property 1.**  $\mu \in C^{\infty}(S_D)$ , where  $S_D = \{S \in \mathbb{R} \mid 0 \le S \le S_m\}$  with  $S_m < \infty$ ; and there exist a value  $S^* \in S_D$  such that  $\mu \le \mu(S^*) \triangleq \overline{\mu} \in \mathbb{R} \ \forall S \in S_D$ , with  $\overline{\mu} < \infty$  as the upper bound of  $\mu$ .

**Property 2.** (Concavity property) The first derivative of  $\mu$  with respect to S, denoted by  $\mu'$  satisfies the follows: (a)  $\mu' > 0 \ \forall \tilde{S} < S^*$ ;  $\mu' = 0$  at  $\tilde{S} = S^*$  and; (b)  $\mu' < 0 \ \forall \tilde{S} > S^*$ , where  $\tilde{S} \in S_D$ 

The aim of this work is to design a robust observer for the estimation of limiting substrate S in anaerobic digestion based only on online measurements for methane outflow rate  $Q_M$ . For

this purpose, we will take into account the dynamics for the methane outflow rate. From (3) we can calculate the time derivative of Q as follows.

$$\frac{dQ_M}{dt} = \dot{Q}_M = k_m(\mu(S)\dot{X} + X\dot{\mu}(S)) = \mu(S)Q_M - \alpha uQ_M + k_mX\dot{\mu}(S)$$

Now from the chain rule we have

$$\dot{\mu}(S) = \frac{d\mu}{dt} = \frac{d\mu}{dS}\frac{dS}{dt} = \mu'(S)(u(S_f - S) - k_t\mu(S)X)$$

where  $\mu'(S) = \frac{d\mu}{dS}$ . By replacing the above expression

$$\dot{Q}_M = (\mu(S) - \alpha u)Q_M + k_m(u(S_f - S) - k_t\mu(S)X)X\mu'(S)$$
(4)

Hence, the modified AD model is given by

$$\dot{S} = u(S_f - S) - k_t \mu(S) X \tag{5}$$

$$\dot{X} = \mu(S)X - \alpha uX \tag{6}$$

$$\dot{Q}_{M} = (\mu(S) - \alpha u)Q_{M} + k_{m}(u(S_{f} - S) - k_{t}\mu(S)X)X\mu'(S)$$
(7)

**Remark 1.** The modified AD model (5-7) admits operational equilibria (different to washout) given by

$$\begin{split} \bar{S} &= \bar{S} \\ \bar{X} &= (\alpha k_t)^{-1} (S_f - \bar{S}) \\ \bar{Q}_M &= k_m (\alpha k_t)^{-1} (S_f - \bar{S}) \mu(\bar{S}) \end{split}$$

where  $\bar{S}$  satisfies  $\mu(\bar{S}) - \alpha u = 0$ .

We can write (5-7) as a nonlinear single output system of the form

$$\dot{x} = f(x, u) \tag{8}$$

$$y = Cx \tag{9}$$

where  $x = (S, X, Q_M)' \in \mathbb{R}^3_+$  is the vector of dynamic states; the vector field  $f : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$  is defined as

$$f(x,u) = \begin{bmatrix} u(S_f - x_1) - k_t \mu(x_1) x_2 \\ \mu(x_1) x_2 - \alpha u x_2 \\ (\mu(x_1) - \alpha u) x_3 + k_m (u(S_f - x_1) - k_t \mu(x_1) x_2) x_2 \mu'(x_1) \end{bmatrix}$$
(10)

and C = [0, 0, 1] such that  $y = Cx = x_3 = Q_M$ .

#### 2.1. On the observability

In order to give a background to the algebraic differential observability used in this contribution the following definitions are considered (Aguilar-López, 2003; Diop & Fliess, 1991; Fliess, 1990).

A differential field *K* is a commutative field of characteristic zero, which is equipped with a single derivation  $\frac{d}{dt}: K \to K$  such that, for any  $a, b \in K$ ,  $\frac{d}{dt}(a+b) = \dot{a} + \dot{b}$  and  $\frac{d}{dt}(ab) = \dot{a}b + a\dot{b}$ . A constant of *K* is an element  $c \in K$  such that  $\dot{c} = 0$ .

A differentiable field extension L/K is given by two differential fields K, L, such that the derivation of  $K \subseteq L$  is the restriction to K of the derivation of L. An element of L is said to be differentially algebraic over K if, and only if, it satisfies an algebraic differential equation with coefficients in K. The extension L/K is said to be differentially algebraic if, and only if, any element of L is differentially algebraic over K.

*Notation.* We denote  $K\langle \kappa \rangle$ , where  $\kappa$  is a subset of the differentiable subfield generated by K and  $\kappa$ .

A ground field is a field k which is fixed in a given situation, such that everything takes place "over" k. Let k be a given differential ground field as a field of functions. A system is a finitely generated differential extension K/k. A dynamics is a system where a finite subset  $u = (u_i, ..., u_m) \subset K$  of control variables has been distinguished, such that the extension  $K/k\langle u \rangle$ is differentially algebraic. An input-output systems is a dynamics where a finite subset  $y = (y_1, ..., y_p) \subset K$  of output variables has been distinguished. This means that any element of K satisfies a differential-algebraic equation with coefficients, which are rational functions over  $k\langle u, y \rangle$  in the components of u, y and a finite number of their time derivatives.

Then an element  $\chi$  in K is said to be algebraically observable with respect to  $\{u, y\}$  if it is algebraic over the differentiable field  $k\langle y, u \rangle$ .

**Definition 1.** (*Fliess, 1990*) A system variable  $\chi \in K$  is said to be algebraically observable if, and only if, it is algebraic over  $k\langle y, u \rangle$ , so that  $\chi$  satisfies a differential polynomial in terms of u, y and some of its time derivatives, i.e.,

$$P(\chi, u, \dot{u}, ..., u^{(k)}, y, \dot{y}, ..., y^{(l)}) = 0$$

with coefficients over  $k\langle y, u \rangle$ .

The above definition is called the Algebraic Observability Condition (AOC) and means that any state variable is algebraic over  $k\langle y, u \rangle$ , i.e., is an algebraic function of the components of u, y and of a finite number of their derivatives. It is known that this definition is equivalent to the classic observability rank condition for systems of the form (8-9)(see Fliess (1990)).

In order to analyze the AOC condition for the system (8-9) we should find a differential polynomial in terms of x, u, y and their time derivatives. From (1)-(3) and (9) it is easy to see that a differential equation of lowest order of  $x_1$  is the following

$$\dot{x}_1 - S_f u + x_1 u + \frac{k_t}{k_m} y = 0$$
(11)

which shows that it is possible estimate  $x_1$  while its dynamics remains stable in terms of u, y and their time derivatives. In previous works (Lara-Cisneros et al., 2012) has been shown that the nominal two-dimensional system (1-2) admits a locally stable nontrivial equilibrium for  $\alpha u < \bar{\mu}$  (with  $\bar{\mu}$  defined in Property 1). Now, by exploiting the cascade structure of the modified version for AD model (8) we can ensure that the system will be locally stable if  $\alpha u < \bar{\mu}$ . Then the following assumption is formulated.

**Assumption 1.** The dilution rate u remains at the bounded interval  $0 < u < \alpha^{-1}\bar{\mu}$ .

Hence, under Assumption 1, we can say that the concentration  $x_1 = S$  is detectable with respect to the pair *u*, *y* defined in (8-9).

#### 3. Observer design

Let us consider the uncertain AD model of the form

$$\dot{x} = f(x, u) + \Delta f$$
(12)  

$$y = Cx$$
(13)

where  $x \in \mathbb{R}^3_+$  is the state vector defined in (8-9) with  $u \in \mathbb{R}$  and  $y \in \mathbb{R}$ ; f(x, u) is the nominal vector field (10),  $\Delta f$  represent an uncertain term related with unmodeled dynamics and load disturbances. Now, we will consider a class of robust observer with a sigmoid-type output injection (Aguilar-López et al., 2014; Gómez-Acata et al., 2015; López-Pérez et al., 2013; Neria-González et al., 2011). For this, we will consider the following assumptions:

**Assumption 2.** The uncertain term  $\Delta f : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$  given by  $\Delta f = [\Delta f_1, \Delta f_2, \Delta f_3]^T$  is bounded in the sense that  $||\Delta f_i|| \le \Xi_i$  with  $0 < \Xi_i < \infty$  for i = 1, 2, 3.

**Assumption 3.** The nominal vector field (10) is locally Lipschitz with respect to x, i.e.,  $||f(x, u) - f(\hat{x}, u)|| \le L||x - \hat{x}||$  with  $L < \infty$ ; and uniformly bounded with respect to u.

**Proposition 1.** The following dynamical system is an observer for the system (12-13)

$$\dot{\hat{x}} = f(\hat{x}, u) + k_l(y - \hat{y}) + k_d \tanh[\gamma(y - \hat{y})]$$
(14)

where  $\hat{x} \in \mathbb{R}^3$  is the estimation vector,  $\hat{y}$  is the estimation value for the output signal,  $\gamma > 0$  and  $k_l, k_d \in \mathbb{R}^3$  are the vectors of observer gains.

*Proof*: In order to show the convergence of the observer (14) we define the following estimation error as

$$e = x - \hat{x}$$

the dynamics for the estimation error is given by

$$\dot{e} = f(x, u) - \bar{f}(\hat{x}, u) + \Delta f - k_l C e - k_d \tanh(\gamma C e)$$
(15)

where  $Ce = y - \hat{y}$ . The following candidate Lyapunov function is proposed as

$$V(e) = e^T Q e \tag{16}$$

with  $Q \in \mathbb{R}^{3x3}$  is a symmetric positive definite matrix, i.e.,  $Q = Q^T > 0$ , and we denote by  $||x||_Q$ the norm  $(x^T Q x)^{1/2}$  such that  $||x||_Q^2 = x^T Q x$ ,  $\Rightarrow ||x||_Q = (x^T Q x)^{1/2}$ . Now, the time derivative of V(e) along the trajectories of (15) is

$$\frac{dV}{dt} = \dot{V}(e) = e^T Q \dot{e} + \dot{e}^T Q e$$

replacing (15) we have

 $\dot{V} = e^T Q[f(x, u) - f(\hat{x}, u) + \Delta f - k_l Ce - k_d \tanh(\gamma Ce)] + [f(x, u) - f(\hat{x}, u) + \Delta f - k_l Ce - k_d \tanh(\gamma Ce)]^T Qe$ Since Q is a symmetric matrix, it follows

$$\dot{V}(e) = 2e^{T}Q[f(x,u) - f(\hat{x},u) + \Delta f] - 2e^{T}Q[k_{l}Ce + k_{d}\tanh(\gamma Ce)]$$
(17)

The symmetric matrix Q can be expressed as  $Q = MM^T$ , then the norm  $||e^T Q[f(x, u) - f(\hat{x}, u)]|| = ||e^T MM^T[f(x, u) - f(\hat{x}, u)]|| = ||\tilde{e}^T \tilde{f}||$ where  $\tilde{e}^T = e^T M$  and  $\tilde{f} = M^T[f(x, u) - f(\hat{x}, u)]$ . In this way, we can define the following norm

$$\|\tilde{e}^T\| = (\tilde{e}^T \tilde{e})^{1/2} = (e^T M M^T e)^{1/2} = (e^T Q e)^{1/2} = \|e\|_Q$$

In the same manner, the following norm is defined  $\|\tilde{f}\| = ([f(x, u) - f(\hat{x}, u)]^T M M^T [f(x, u) - f(\hat{x}, u)])^{1/2} = ([f(x, u) - f(\hat{x}, u)]^T Q [f(x, u) - f(\hat{x}, u)])^{1/2} = \|f\|_Q$ 

By applying the Cauchy-Schwarz inequality it follows  $\|e^T Q[f(x, u) - f(\hat{x}, u)]\| = \|\tilde{e}^T \tilde{f}\| \le \|\tilde{e}\| \|f\| = \|e\|_Q \|f\|_Q$ 

$$\Rightarrow \|e^{T}Q[f(x,u) - f(\hat{x},u)]\| \le \|e\|_{Q}\|f\|_{Q}$$

And similarly,  $||e^T Q \Delta f|| = ||\tilde{e}^T \Delta \tilde{f}|| \le ||\tilde{e}||||\Delta \tilde{f}|| = ||e||_Q ||\Delta f|_Q$ 

$$\Rightarrow \|e^T Q \Delta f\| \le \|e\|_Q \|\Delta f\|_Q \tag{19}$$

(18)

In the same manner

 $||e^T Q[k_d \tanh(\gamma C e)]|| = ||\tilde{e}\tilde{\varphi}||$ 

where  $\tilde{e} = e^T M$  and  $\tilde{\varphi} = M^T [k_d \tanh(\gamma C e)]$ . It follows that

$$\|e^T Q[k_d \tanh(\gamma C e)]\| \le \|e\|_Q \|k_d \tanh(\gamma C e)\|_Q$$
(20)

and similarly

$$|e^T Q[k_l Ce]|| \le ||e||_Q ||k_l Ce||_Q$$

with  $||k_l C e||_Q = ([k_l C e]^T Q[k_l C e])^{1/2}$ . By considering a matrix norm, it follows that

$$\|e^{T}Q[k_{l}Ce]\| \le \|k_{l}C\|_{\infty} \|e\|_{Q}^{2}$$
(21)

where  $||k_l C||_{\infty}$  is the matrix norm defined as the maxumum row sum of the matriz  $k_l C \in \mathbb{R}^{3X3}$ . In this way, from (18)-(21)

$$\dot{V}(e) \le 2[||f||_{Q}||e||_{Q} + ||\Delta f||_{Q}||e||_{Q} - ||k_{l}C||_{\infty}||e||_{Q}^{2} - ||k_{d}\tanh(\gamma C e)|||e||_{Q}]$$

From the Assumption 3, we have

$$\|f\|_{Q} = \|f(x,u) - f(\hat{x},u)\|_{Q} \le L\|x - \hat{x}\| = L\|e\|_{Q}$$
$$\|f\|_{Q} \le L\|e\|_{Q}$$
(22)

Now, from Assumption 2,  $||\Delta f_i|| \le \Xi_i$  for i = 1, 2, 3, and since  $|| \tanh(\gamma C e) || \le 1$  we have

$$||k_d \tanh(\gamma C e)|| \le ||k_d||$$

Thus,

$$\dot{V}(e) \le 2[(L - ||k_l C||_{\infty})||e||_Q^2 + ||\Xi - k_d||||e||_Q]$$
(23)

where  $\Xi = (\Xi_1, \Xi_2, \Xi_3)$ . Now by applying the Lyapunov stability criteria, the vectors of observer gains  $k_l$  and  $k_d$  should be chosen in order to keep  $\dot{V}(e) \leq 0$ . Furthermore, getting back to the

estimation error dynamics (15), and taking into account the *Q* norm defined above, it follow that  $V(e) = e^T Q e = ||e||_Q^2$ . Then, if we calculate the derivative with respect to the time

$$\frac{dV(e)}{dt} = \frac{d||e||_Q^2}{dt} = 2||e||_Q \frac{d||e||_Q}{dt}$$

From (23) it follows

$$2||e||_{Q} \frac{d||e||_{Q}}{dt} \leq 2[(L - ||k_{l}C||_{\infty})||e||_{Q}^{2} + ||\Xi - k_{d}|||e||_{Q}]$$

then

$$\frac{d||e||_Q}{dt} \le (L - ||k_l C||_{\infty})||e||_Q + ||\Xi - k_d||$$
(24)

The solution of the differential inequality (24) satisfies

$$\|e(t)\|_{Q} \le \|e_{0}\|_{Q} \exp\left(L - \|k_{l}C\|_{\infty}\right)t + \frac{\|\Xi - k_{d}\|}{L - \|k_{l}C\|_{\infty}} \left[1 - \exp\left(L - \|k_{l}C\|_{\infty}\right)t\right]$$
(25)

where  $e_0 = e(0)$ . Hence, when  $t \to \infty$  the norm of the estimation error  $||e(t)||_Q \to \frac{||\Xi - k_d||}{L - ||k_t C||_{\infty}}$ , or

$$\lim_{t \to \infty} ||e(t)||_Q \le (L - ||k_l C||_{\infty})^{-1} ||\Xi - k_d||$$

Therefore, in order to provide a small enough estimation error the following must be ensured  $(L - ||k_lC||_{\infty}) \gg ||\Xi - k_d||$  or  $||e||_Q \sim 0$  if  $||\Xi - k_d|| \sim 0$ , these can be ensured with an appropriate choice of  $k_l$  and  $k_d$ .  $\Box$ 

#### 4. Numerical verification

The aim of this section is to illustrate the performance of the robust observer (14) by numerical simulations using a more realistic AD model with two degradation stages (acidogenic and methanogenic degradation) for the soluble substrate and will be considered fluctuations in the inlet composition. For this purpose the AD model developed in Bernard et al. (2001) is considered. The underlying model assumes two main bacterial populations, the first one, called acidogenic bacterial  $X_1$ , consumes organic substrate  $S_1$  (total soluble Chemical Oxygen Demand COD except Volatile Fatty Acids VFA) and produces VFA, that is considered as secondary substrate  $S_2$  through an acidogenesis stage. The second population, known as methanogenic bacteria  $X_2$ , uses VFA as substrate in a methanogenesis stage for growth and produces methane and carbon dioxide. Thus, the global anaerobic process can be written as the reduced biochemical reaction network

$$k_1 S_1 \stackrel{\mu_1(\cdot)X_1}{\hookrightarrow} X_1 + k_2 S_2 \tag{26}$$

$$k_3 S_2 \stackrel{\mu_2(\cdot)X_2}{\hookrightarrow} X_2 + k_4 C H_4 \tag{27}$$

It is important to note that unlike to the one-stage degradation model (1-2), in Bernard et al. (2001) it is considers two degradation stages for the soluble organic substrate as the two bioreaction (26-25). Hence, the corresponding mass-balance for a continuous anaerobic process it

reads:

$$\dot{S}_1 = D(S_{1f} - S_1) - k_1 \mu_1(S_1) X_1$$
 (28)

$$\dot{X}_1 = \mu_1(S_1)X_1 - \alpha DX_1$$
(29)

$$\dot{S}_2 = D(S_{2f} - S_2) + k_2 \mu_1(S_1) X_1 - k_3 \mu_2(S_2) X_2$$
(30)

$$\dot{X}_2 = \mu_2(S_2)X_2 - \alpha DX_2$$
 (31)

Similarly, in Bernard et al. (2001) the outflow rate of methane gas  $Q_M$  proportional to the reaction rate of the methanogenesis stage

$$Q_M(\xi) = k_4 \mu_2(S_2) X_2 \tag{32}$$

where  $k_4$  is the yield coefficient for the methane production. With respect to the specific growth rates for the acidogenic and methanogenic populations, in Bernard et al. (2001) are assumed to be described by the Monod and Haldane expressions, respectively, i.e.,

$$\mu_1(S_1) = \frac{\mu_{1,max}S_1}{K_{S1} + S_1} \tag{33}$$

$$\mu_2(S_2) = \frac{\mu_{2,max}S_2}{K_{S2} + S_2 + S_2^2/K_{I2}}$$
(34)

where  $\mu_{1,max}$ ,  $K_{S1}$ ,  $\mu_{2,max}$ ,  $K_{S2}$ , and  $K_{I2}$  are the maximum bacterial growth rate and the halfsaturation constant associated to the substrate  $S_1$ , the maximum bacterial growth rate in the absence of inhibition, and the saturation and inhibition constants associated to substrate  $S_2$ , respectively.

For numerical simulations the nominal parameter values reported in Bernard et al. (2001) have been used (see Table 1). It is important to remark the following: the observer (14) only requires a nominal vector field as has been explained in Section 2, i.e., the nominal vector field (10) is described by a single degradation stage with constant inlet composition (see Section 2). The parameter values used for the nominal vector field (10) are set as  $k_t = k_3$ ,  $k_m = k_4$  and  $\mu(\cdot) = \mu_2(S_2)$  with  $S = S_2$ . The observer gain vectors are set to the following values:  $k_l = (-2, 0.1, 0.1)^T$  and  $k_d = (-1, 0.1, 0.1)^T$  with  $\gamma = 15$ .

The performance of the proposed estimation methodology is shown in the Fig. 2 with disturbances in the inlet composition (see Fig. 1). A comparison with a local Luenbergertype observer was done to show the robustness of the proposed observer despite of changes in the operative conditions. The tuning methodology for the Luenberger-like observer is based on a local linearization at the nominal equilibrium  $\bar{S} = 4.0, \bar{X} = 0.5672, \bar{Q}_M = 2.2310$  and  $\bar{u} = 1.0174$ , using the pole placement technique with p = (-1, -1, -2), then the observer's gains are  $k = (8.72, -3.29, 3.89)^T$ . In the Fig 2b, we can see that the local performance of the Luenberger-type observer is more close to the actual VFA concentration. It is important to note that the best performance of the Luenberger-type observer is only locally around of the operating conditions where it was designed (see Fig. 3). It is well known that the main drawback of the local observers approaches is their poor performance for operating condition far from of the designed conditions, mainly for strong nonlinear and intrinsically unstable systems. As it can be see the Luenberger-type observer exhibit large overshoots and longer setting times for different operating conditions. In contrast, the proposed robust estimation methodology is able to compensate unmodeled dynamics and load disturbances for different operating conditions which lead to more satisfactory performance for the estimation of VFA concentration. With respect to the

Parameter	Value	Units	
$k_1$	42.14	g/g	
$k_2$	116.5	mmol/g	
$k_3$	268	mmol/g	
$k_4$	453	mmol/g	
$\mu_{1max}$	0.05	$h^{-1}$	
$\mu_{2max}$	0.031	$h^{-1}$	
$K_{S1}$	7.1	g/L	
$K_{S2}$	9.28	mmol/L	
$K_{I2}$	16	mmol/L	
α	0.5		
$S_{1f}$	10	g/L	
$S_{2f}$	80	mmol/L	

Table 1: Nominal parameter values used in the numerical simulations (Bernard et al., 2001).

estimation of the concentration for the methanogenic bacteria, in Fig. 4 is shown the performance of the proposed observer for the estimation of  $X_2$ . Also, it shown a better estimation with respect to the Luenberger-type observer with changes in the operating conditions for AD process. The performance of the proposed observer for parametric variations ( $\pm 5\%$ ) in the nominal values for the simplified model using for the observer design (8-10) is shown in Fig. 6 Finally, in order to illustrate the effect of the measurement noise, numerical simulations are performed assuming that the methane outflow rate  $Q_M$  is corrupted by additive noise. In Fig. 5 an acceptable performance of the proposed estimation method is shown in presence of measurement noise. In the context of experimental implementation of the proposed estimation methodology there is a need a more exhaustive analysis of the observer convergence in order to provide a tuning methodology for the observer gain vectors ( $k_l, k_d$ ).

#### 5. Conclusion

In this paper we have designed a robust nonlinear observer for the online estimation of Volatile Fatty Acids (VFA) concentration, as a key variable in Anaerobic Digestion process, only from methane outflow rate measurements. The observer is based on a modified version for a simple AD model by including the dynamics for the methane production. It is shown that the observer structure composed by a linear with a sigmoid injection terms is able to reject unmodeled dynamics and load disturbances in AD process. Unlike to the local observers, the proposed observer is able to the VFA estimation in different operation conditions.

The study of a tuning methodology for the observer's gains based on an exhaustive convergence analysis in the context of experimental implementation, need to be looked into more deeply.

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(a)



Figure 1: Load disturbances in the inlet composition, with  $S_{1f}[gL^{-1}]$  and  $S_{2f}[mmolL^{-1}]$ .

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Figure 2: Performance of the proposed estimation methodology with load disturbances in the inlet composition.

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Figure 3: Window of the Fig. 2 for the interval of 30 to 50 days.

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Figure 4: Performance of the proposed observer for the estimation of methanogenic bacteria.

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Figure 5: Observer performance with additive noise in the measurable signal  $y = Q_M$ .



Figure 6: Observer performance with parametric variations ( $\pm 5\%$ ) in the nominal values for the simplified model using for the observer design (8-10).