

# Technical Report

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## Nonlinear model of leachate anaerobic digestion treatment process

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## Abstract

In this report a continuous adaptive high-gain observer method is presented for the estimation of state variables that could not be measurable online and unknown time-varying parameters of leachate anaerobic digestion treatment process. The high-gain observer is a variant of the Luenberger extended observer and involves an adjustable gain parameter. It is characterized by easy implementation and calibration, is stable and exhibit exponential convergence. The observer is based on a simplified mathematical model of the system. Calibration of the model was performed with real data from the Upflow Anaerobic Sludge Blanket (UASB) reactor for landfill leachate treatment in open loop under normal operational conditions. The model performance is evaluated via numerical simulations showing adequate results. The criteria used for considering the model as acceptable is to calculate the values of Mean Magnitude of Relative Error (MMRE) and Prediction at level  $l$ .

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## 1 Introduction

Determining a mathematical model to represent bioprocess behaviour is a difficult issue, mainly because of the complexity inherent to biological systems [8]. For example, in an anaerobic digestion bioprocesses for wastewater treatment, the main operational problems are associated to its highly nonlinear behaviour, load disturbances, system uncertainties, limited online measurement information and constraints on manipulated and state variables [41, 46]. The measurement of variables and parameters online is difficult because of the absence of proper instrumentation, due to its high cost or unavailability. Also, these processes have infinitely many parameter sets that produce exactly the same output for every input and thus the model parameters cannot be estimated from any experimental measurements.

In this work is proposed to use a nonlinear observer based on mathematical model of the system to describe the dynamics of continuous landfill leachate anaerobic digestion process from the measurement of some variables. An adaptive high-gain observer for the estimation of non-measurable state variables online and time-varying parameters. The observability problem consists in investigating whether there exist relations binding the state variables to the inputs, the outputs and their time derivatives and thus locally defining them uniquely in terms of controllable/measurable quantities without the need for knowing the initial conditions. If no such relations exist, the initial state of the system cannot be deduced from observing its input-output behaviour [3].

A method of adaptive high-gain observer type is used, which could be easily calibrated because it has only one tuning parameter and does not require any additional equation to calculate it, as is the case of extended Kalman observers in which to calculate the tuning parameters of the observer requires solving a dynamic equation [22].

The observer is designed based on a simplified anaerobic digestion phenomenological model. Some studies have shown that simple models can accurately represents the main system features such as presented by Bernard et.al., 2005 [8]. Due to the complexity of the anaerobic process in which a great number of bacterial populations intervene, it is assumed that the dynamics of the system presents two main stages: acidogenesis and methanogenesis [7]. Numerical simulations with real data obtained from the Upflow Anaerobic Sludge Blanket (UASB) reactor in open loop under normal operating conditions were performed.

Results show that the nonlinear observer designed based on phenomenological model to estimate variables state and time-varying parameters unknown is the model that has a better performance in order to describe the dynamic behaviour of the UASB reactor to leachate anaerobic digestion process. The criteria for comparing the models designed corresponds to compute the Mean Magnitude of Relative Error (MMRE) and Prediction at Level  $l$ ,  $\text{-PRED}(l)$  [20].

The remainder of this document is divided into five sections. The first section presents a review of the state of the art followed by the theoretical framework in the Section II. The case of study is showed in Section III. Then, Section IV presents preliminary results of the performance models. Finally, conclusions are presented in Section V.

## 2 Background

First works developed to states estimation were presented by Kalman in 1960 [29] and Luenberger in 1971 [33], for linear systems based on the observability property. However, observable property of a nonlinear system depends on the inputs of the same, therefore, for non-linear systems, there is no general solution.

The design of nonlinear observers has been a very active research area [19], particularly from the seventies with the works presented by Krener and Isidori in 1983 [31], Krener and Respondek in 1985 [32], Marino in 1990 [34] and Deza in 1993 [17]. Extended Kalman observers (Extended

Kalman Filter or EKF) [11], extended Luenberger observers [49] and nonlinear high-gain observers [24, 47] are the observers more used to estimate state variables for nonlinear systems in the automatic control field.

One problem with the above observers is that the theory for the extended Luenberger and Kalman observers and for the nonlinear observers is developed using perfect knowledge of the system parameters, in particular of the process kinetics. It is difficult to develop error bounds and there is often a large uncertainty on these parameters, being one major challenge that parameter and state estimators applied to chemical and biochemical processes, including the model and measurement uncertainties [19].

In the observer designing, model uncertainties are mainly due to parameters unknown, difficult to measure or physically unmeasurable [22]. An alternative to solve this problem is the use of adaptive observers, which perform state variables and parameters estimation in a dynamic system simultaneously.

Adaptive observers have been used successfully in a wide variety of chemical engineering processes. Some applications are: adaptive robust observers for non-linear uncertain systems [14], asymptotic observers for stirred tank reactors [16], an adaptive high-gain observer applied to a bioreactor [12], estimation of the glass transition temperature of free-radical copolymers [23], on-line estimates of the number of moles of each polymerizing species in the reactor and the state estimator provides a value for a lumped kinetic parameter proportional to the product [45], on-line growth rates parameter estimation in bioprocesses [42], state estimation for bioprocesses [18], state variables and lumped parameter associated to the number of moles of radicals per liter of emulsion estimation in polymerization reactors [4], estimates the overall heat transfer coefficient of heat exchangers [5], among others.

Specifically in biochemical processes, the idea of the asymptotic observers is to take advantage of the structure of the dynamical models to rewrite part of the model in a form independent of the process kinetics. The asymptotic observers belong indeed to the class of observers for systems with unknown inputs, the unknown input being here the process kinetics [19].

### 3 Nonlinear high-gain observer

Observability is a structural property of a control system defined as the possibility to estimate the state variables of the system from observing its input-output behaviour [3]. Consider the general continuous time system,

$$(S) \begin{cases} \dot{x}(t) = f(x(t), u(t)); & x(t_0) = x_0, \\ y(t) = h(x(t)), \end{cases} \quad (1)$$

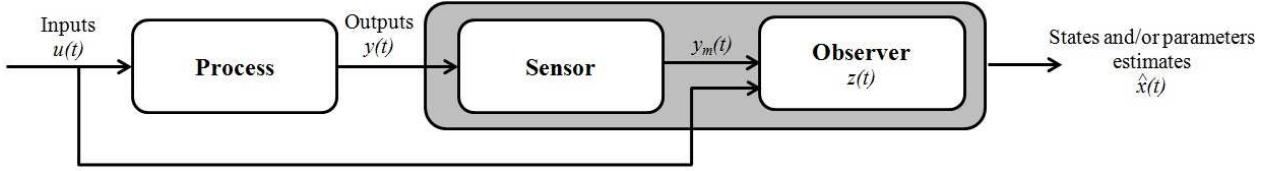
where,  $x \in \mathbb{R}^n$  is the state-space vector,  $u \in \mathbb{R}^m$  is the input vector,  $y \in \mathbb{R}^p$  is the output vector,  $x_0$  is the initial conditions for the initial time,  $f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$  and  $h : \mathbb{R}^n \rightarrow \mathbb{R}^p$  [18].

Assuming that for the system (1) the input  $u(t)$  and the output  $y(t)$  are known, and the functions  $f$  and  $h$  are known from phenomenological model, and considering the following definitions from [26, 18, 24]. In general, for nonlinear systems, the observability depends on the input; a system can be observable for some inputs and not observable for others. For any input, the initial condition can be uniquely estimated from the output [9]. If all the inputs are universal, the system is uniformly observable and can be rewritten under specific form. The notion of universal input is defined as an input for which every pair of initial states can be distinguished by observation of the output [10].

**Definition 1.** *Two states  $x_0$  and  $x'_0$  are said to be indistinguishable, if for any input time function  $u(t)$  and for any  $t \geq 0$ , the outputs  $h(x(t, x_0))$  and  $h(x(t, x'_0))$  are identical for any  $t \geq 0$ .*

**Definition 2.** *The system (1) is said observable if it does not have any distinct couples of initial state  $x_0$  and  $x'_0$ , that are indiscernible.*

Figure 1 shows the nonlinear observer principle, where  $\hat{x}(t)$  is the state and/or parameter estimate vector by the observer and  $y_m(t)$  is the measured output. The observer is based on a phenomenological model of the system.



**Figure 1:** Observer principle

### 3.1 Nonlinear continuous high-gain observer to estimate state variables in biological processes

A high-gain observer is designed to state space estimation. The simulation model of the systems with respect to the input, could be described as follow [18, 9]:

$$\dot{x}(t) = f(x(t)) + ug(x(t)). \quad (2)$$

For bioreactors, the input usually corresponds to the dilution rate,  $u = D$ . Moreover, assumed that the output is a function of the state,

$$y(t) = h(x(t)). \quad (3)$$

Making a change of coordinates or an original system transformation,  $z = \phi(x)$ ,

$$\phi(x) = \begin{bmatrix} h(x) & L_f h(x) & \cdots & L_f^{n-1} h(x) \end{bmatrix}^T, \quad (4)$$

where,  $L_f h(x) = \frac{\partial h}{\partial x} f(x)$  denotes the Lie derivative of  $h(x)$  along the vector  $f$ .

*Uniformly observable* nonlinear systems [24] have the property of transforming the original system by a change of coordinates into triangular form

$$\begin{aligned} \dot{z}(t) &= Az(t) + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \varphi(z(t)) \end{bmatrix} + \psi(z(t)u(t)), \\ y(t) &= Cz(t), \end{aligned} \quad (5)$$

where,

$$A = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ \vdots & & & \ddots & 1 \\ 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix}, C = [1, 0, \dots, 0],$$

$$z(t) = \begin{bmatrix} h(x) & L_f h(x) & \cdots & L_f^{n-1} h(x) \end{bmatrix}^T,$$

$$\psi(z(t)) = \begin{bmatrix} \psi_1(z_1(t)) \\ \psi_2(z_1(t), z_2(t)) \\ \vdots \\ \psi_n(z_1(t), z_2(t), \dots, z_n(t)) \end{bmatrix},$$

with

$$\psi_i(z(t)) = L_g L_f^{(i-1)} h(\phi^{-1}(x(t))).$$

The triangular form (5) is used to design an exponential observer. The structure of this observer takes the following form:

$$\dot{\hat{x}}(t) = f(\hat{x}(t)) + g(\hat{x}(t))u(t) - \left[ \frac{\partial \phi(t)}{\partial x} \right]_{x(t)=\hat{x}(t)}^{-1} S_\theta^{-1} C^T [h(\hat{x}(t)) - y(t)], \quad (6)$$

where,  $\hat{x}$  is the estimate value and  $S_\theta^{-1}$  is the solution of the Lyapunov algebraic equation  $\theta S_\theta + A^T S_\theta + S_\theta A = C^T C$ , where  $\theta > 0$  is a high gain fixed parameter, A and C are as above, and  $S_\theta$  can be calculated as follows:

$$S_\theta(i, j) = \frac{(-1)^{i+j} (i+j-2)!}{\theta^{i+j-1} (i-1)! (j-1)!}. \quad (7)$$

### 3.2 Nonlinear observers to estimate state variables and unknown and time-varying parameters estimation in biological processes

In this case, the parameters are considered state variables with time derivative zero. Therefore, biological process is formulated in a state-space model as shown below.

$$\begin{aligned} \dot{p} &= 0, \\ \dot{x} &= f(x, p, u), \\ y &= h(x, p). \end{aligned} \quad (8)$$

The simulation model of the systems with respect to the input, could be described as follows:

$$\dot{x}(t) = p(t)\bar{f}(x(t)) + ug(x(t)) \quad (9)$$

where,  $p$  is the parameter time-varying vector and corresponds to the maximum growth rate. Observer designed is an extension of the observer to a system of the form (8) and the behaviour of the parameter time-varying can be modelled using

$$p(t) = \zeta(t), \quad (10)$$

where,  $\zeta(t)$  is any bounded function [23, 4]. Performing change of coordinates,  $\bar{z} = \bar{\phi}(x)$ ,

$$\bar{\phi}(x) = \begin{bmatrix} h(x) & L_{\bar{f}} h(x) & \cdots & L_{\bar{f}}^{n-1} h(x) \end{bmatrix}^T, \quad (11)$$

where,  $L_{\bar{f}} h(x) = \frac{\partial h}{\partial x} \bar{f}(x)$  denotes the Lie derivative of  $h(x)$  along the vector  $\bar{f}$ .

This transforms the original system into the following triangular form:

$$\begin{aligned} \dot{\bar{z}}(t) &= \zeta(t) A \bar{z}(t) + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \varphi(\bar{z}(t)) \end{bmatrix} + \psi(\bar{z}(t))u(t), \\ y(t) &= C \bar{z}(t). \end{aligned} \quad (12)$$

For this system, the observer is given by

$$\begin{aligned}\dot{\hat{x}}(t) &= \hat{\zeta} \bar{f}(\hat{x}(t)) + g(\hat{x}(t))u(t) - \left[ \frac{\partial \bar{\phi}}{\partial x(t)} \right]_{x(t)=\hat{x}(t)}^{-1} \Gamma S_{\theta}^{-1} C^T (h(\hat{x}(t)) - y(t)), \\ \dot{\hat{\zeta}}(t) &= -\frac{\theta^2}{\hat{\varphi}(t)} [h(\hat{x}(t)) - y(t)],\end{aligned}\quad (13)$$

where,

$$\Gamma = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & \frac{1}{\hat{\zeta}(t)} & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \frac{1}{\hat{\zeta}(t)^{n-2}} & 0 \\ 0 & 0 & \cdots & 0 & \frac{1}{\hat{\zeta}(t)^{n-1}} \end{bmatrix}. \quad (14)$$

For the convergence proof and further details see [18, 24, 4].

## 4 Case study: Application to anaerobic digestion leachate treatment process

The leachate from landfill is a liquid generated mainly by the breakdown of waste in the landfill, rainwater percolation, and inherent moisture content of the wastes [21, 30, 43]. Landfill leachate contains a variety of contaminants including organic matter, ammonium nitrogen, inorganic compounds, chlorinated organic, inorganic salts, heavy metals and toxic materials such as xenobiotic organic substances [1, 43, 50]. It possesses high values of biological oxygen demand (BOD) and chemical oxygen demand (COD)[48].

Accurate prediction of the composition of landfill leachate, over the life of a landfill is problematic [21]. The composition of leachate varies due to variations in waste composition, complex chemical and biological processes occurring within the landfill, landfill hydrology, landfill age, engineering and climate [1, 21, 50]. Also, the composition of the leachate differs between the outside points from same landfill.

Commonly, the landfill leachate is classified with age into three stages: young (less than 5 years), medium (5–10 years), and old (more than 10 years). The ratio BOD/COD is commonly recognized to be the most representative property of landfill leachate age because it is directly related to the biodegradability of leachate. The BOD/COD ratios of young, medium, and old leachate are in the ranges of 0.5–1.0, 0.1–0.5, and less than 0.1, respectively [1]. Toxicity analysis has been demonstrated that this liquid is highly toxic and represent an environmental problem because can pollute the land, ground water and water ways. It is mandatory for landfills implement a treatment system to reduce the pollutant loading and comply with certain discharge to the receptor medium [30, 48]. The removal of organic material based on chemical oxygen demand (COD), biological oxygen demand (BOD) and ammonium from leachate is the usual prerequisite before discharging the leachates into natural waters [43].

Many treatment processes have been studied to control the pollution caused by landfill leachate. For example, biological treatment processes, including anaerobic and aerobic processes, are quite effective and the most economical way to treatment for young landfill leachate with a high BOD<sub>5</sub>/COD [48, 50]. In this work, is presented the anaerobic digestion process to landfill leachate treatment from Manizales. Due to the difference of composition between old and young landfill leachate, these are mixed in a homogenizer before entering to UASB reactor. At the entrance of the reactor, it has 0.5 BOD/COD average ratio and significant concentrations of biodegradable organic matters such as volatile fatty acids (VFA).

The UASB reactor has two units, each with a capacity of 90 m<sup>3</sup>. Flow is distributed uniformly

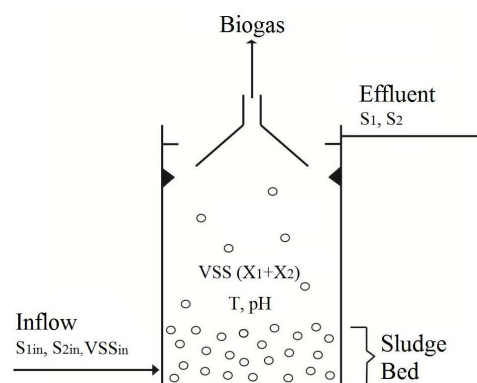
to each unit of an upper trough equipped dumps and it feeding the delivery side flow pipes at bottom of the reactor. The reactor is designed at hydraulic retention time of 24 hours, for a maximum total flow of 2 L/s.

The reactor has a system that ensures partial sludge blowdown and coring. The effluent is collected by a lateral gutter and download in a set of pipes to the outlet chamber, which you can perform volumetric measurement of the overall outflow. Gases generated are conducted from the interior of each reactor to the surface, and these are accumulated in bells that lead to the fireplace, where the gases are burned permanently in order to achieve the destruction of the methane generated [25]. In Figure 2 is shown a typical scheme of an UASB reactor.

Anaerobic digestion is characterized by the existence of several distinct consecutive stages (hydrolysis, acidogenesis and methanogenesis) in the substrate degradation process, intervening five large microbial populations: hydrolytic–acidogenic bacteria, acetogenic bacteria, acetogenic bacteria, hydrogenofile methanogenic bacteria and acetoclastic methanogenic bacteria as shown in Figure 3. These populations are characterized by being composed beings different growth rates and different sensitivities to each intermediate compound (inhibitor). Each stage will present different growth rates depending of the substrate composition and the stability of the global process development with the purpose of avoid the accumulation of inhibitory intermediates or accumulation of volatile fatty acids (VFA), which could cause pH decrease [28].

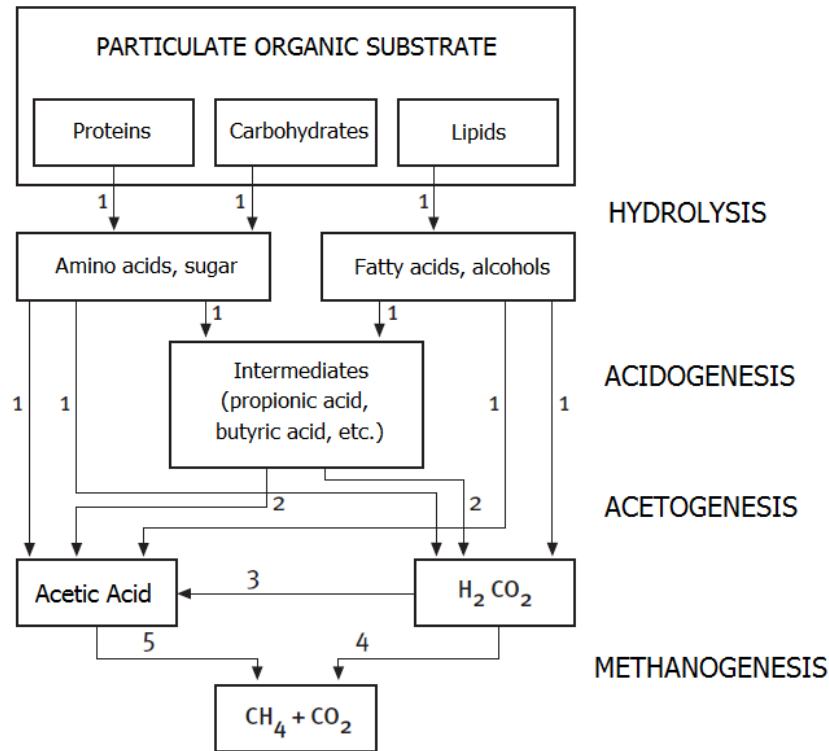
Some factors that affecting the operation in anaerobic digester are [13]:

1. Reactor ability to retain biomass under varying conditions (A higher concentration of active cells retained in the reactor could be treated higher organic loads) and the gas-solid-liquid separation system are the design and operating factors keys in anaerobic reactors.
2. Hydraulic retention time (HRT) should be sufficient to permit close contact between sludge and substrate.
3. Temperature affects the activity and the growth of bacteria (Most of the bioreactors and/or anaerobic digestors operate between 30-35 °C, so that the formation of CH<sub>4</sub> at 20°C is low).
4. Bioreactor must operate between 6.8 and 7.5 pH range, because the methanogenic population activity is highly vulnerable to changes in pH.
5. VFA are toxic to methanogenesis, only in the unionized form and it depends of the pH conditions.
6. Alkalinity/VFA ratio is a useful parameter to VFA accumulation of anaerobic reactors: a



**Figure 2:** A typical anaerobic digester





**Figure 3:** Phases of anaerobic digestion and microbial populations: 1. hydrolytic-acidogenic bacteria, 2. acetogenic bacteria, 3. acetogenic bacteria, 4. hydrogenofile methanogenic bacteria and 5. acetoclastic methanogenic bacteria.

value of 0.2 indicates an excellent buffer system with a maximum value of 0.4, (a value of 0.35 indicates acidification).

#### 4.1 Phenomenological model

To represent the dynamic of the anaerobic process is considered a simplified mathematical model. Assuming that the dynamics of the anaerobic digestion system presents two main stages, acidogenesis and methanogenesis stage, the reactor behaves like a perfectly mixed tank, and the biomass is uniformly distributed within the reactor [7, 18].

- Acidogenesis stage (at rate  $\mu_1$ ):



- Methanogenesis stage (at rate  $\mu_2$ ):



Constants  $k_1$ ,  $k_2$  and  $k_4$  respectively represent stoichiometric coefficients associated with consumption of substrate  $S_1$ , production of VFA and  $CO_2$  in the acidogenesis process.  $k_3$ ,  $k_5$  and  $k_6$  respectively represent stoichiometric coefficients in the consumption of VFA and in the production of  $CO_2$  and  $CH_4$ , during the methanogenesis process.

For bacterial kinetics is considering Monod model [39] for the growth of acidogenic bacteria,

$\mu_1 = \frac{\mu_{1max}S_1}{K_{S1}+S_1}$  and Haldane model [40] for the methanization,  $\mu_2 = \frac{\mu_0S_2}{K_{S2}+S_2+\frac{S_2^2}{K_I}}$ .

The dynamic model that describes the behaviour of the liquid phase is presented below. The model proposed includes the biomass decay rate and the temperature and pH activity coefficient in the growth specific rate.

- Acidogenesis stage

$$\dot{X}_1 = D(X_1^0 - \alpha X_1) + \mu_1 X_1 \Theta^{T-20} I_{pH} - k_d X_1, \quad (17)$$

$$\dot{S}_1 = D(S_1^0 - S_1) - k_1 \mu_1 X_1 \Theta^{T-20} I_{pH}. \quad (18)$$

- Methanogenesis stage

$$\dot{X}_2 = D(X_2^0 - \alpha X_2) + \mu_2 X_2 \Theta^{T-20} I_{pH} - k_d X_2, \quad (19)$$

$$\dot{S}_2 = D(S_2^0 - S_2) + k_2 \mu_1 X_1 \Theta^{T-20} I_{pH} - k_3 \mu_2 X_2 \Theta^{T-20} I_{pH}. \quad (20)$$

Where,  $\theta^{T-20}$  represents the inhibition by temperature [15] and  $I_{pH}$  represents the inhibition by pH [2, 36] and it is expressed as

$$I_{pH} = \frac{1 + 2 * 10^{0.5(pH_{LL}-pH_{UL})}}{1 + 10^{(pH-pH_{UL})} + 10^{0.5(pH_{LL}-pH)}}. \quad (21)$$

Some values of kinetic parameters (See Table 1) are adjusted heuristically based on the ranges and values are reported in the literature [2, 7, 6, 40, 35] and the other values are a set of parameter that minimizes a global criteria based on the error between simulated values and measurements. The identification was done using GAMS [44] and MatLab [37]. Value ranges of state variables and inputs (Table 2) are from historical real data base from UASB reactor in open loop at normal conditions.

## 5 Results

This section presents the results obtained from design of two nonlinear observers as model of anaerobic digestion processes in the UASB reactor to leachate treatment. Assuming that it

**Table 1:** Estimates values of kinetic parameters

Parameter	Meaning	Value
$k_1$	yield for substrate degradation	10.67
$k_2$	yield for VFA production	0.43
$k_3$	yield for VFA consumption	2.12
$\alpha$	proportion of dilution rate for bacteria	0.6
$\mu_{1max}$	maximum acidogenic biomass growth rate	0.2 – 2.5
$\mu_0$	maximum methanogenic biomass growth rate	0.2 – 2.0
$K_{S1}$	half-saturation constant associated with $S_1$	14522
$K_{S2}$	half-saturation constant associated with $S_2$	2507
$K_I$	inhibition constant associated with $S_2$	32.15
$k_d$	biomass decay rate	0.02 <sup>a</sup>
$\theta$	temperature activity coefficient	1.02 – 1.09 <sup>a</sup>

<sup>a</sup> From [40], <sup>b</sup> From [35]

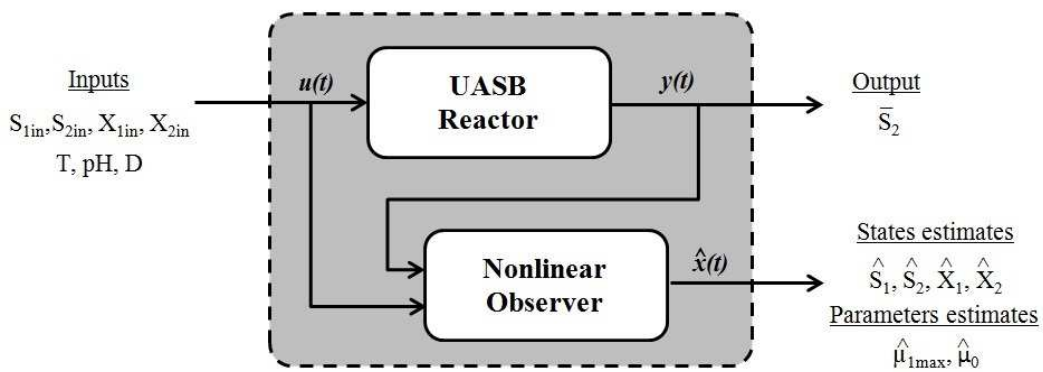
**Table 2:** Values of state variables and inputs

Parameter	Meaning	Range value
pH	potential of hydrogen	7.0 – 8.5
T	temperature ( $^{\circ}C$ )	15 – 25
$T_{ref}$	reference temperature ( $^{\circ}C$ )	20
$S_1$	output organic substrate concentration	3000 – 10000
$S_{1in}$	inlet organic substrate concentration	7000–20000
$S_2$	outlet volatile fatty acids concentration	100–500
$S_{2in}$	inlet volatile fatty acids concentration	400–1200
VSS	volatile suspended solids concentration	100–10000
$VSS_{in}$	inlet volatile suspended solids concentration	100–1000

starts feeding an input  $u$  at time zero when the system is at an unknown state  $x$  and the reactor behavior is observed in terms of the outputs produced [3]. The first observer designed corresponds to a nonlinear observer to estimate states variables from one measurable variable assuming that the parameters are known (Case 1), and the second case corresponds to an adaptive high gain observer to estimated states variables and time-varying and unknown parameters from one measurable variable (Case 2). Figure 4 shows the schematic of the nonlinear observer based on a phenomenological model of the anaerobic digestion process.

Several parameters should be estimated for proper control (volatile acids concentration,  $CO_2$  percentage in gas, pH, total gas production and waste stabilization) in an anaerobic wastewater treatment processes [27]. However, of the many parameters the volatile acids analysis has proven to be one of the most important control test for anaerobic digestion. An increase in the volatile acids concentration is one of the first signs of an upset digester and signals the need of control measures long before a drop in pH. In extreme cases, the efficient could decrease to almost zero and a stuck digester result[38]. For this reason, in this work is assumed the measuring of the concentration of short chain fatty acids which are formed as intermediate products during the anaerobic breakdown of complex organic matter.

The criteria for comparing the model performance on the datasets is computing the values of Mean Magnitude of Relative Error (MMRE) and Prediction at Level  $l$  (PRED)[20].

**Figure 4:** Principle of the nonlinear observer based on a phenomenological model

The MMRE is defined as

$$MMRE = \frac{1}{n} \sum_{i=1}^n \left| \frac{e_i - \hat{e}_i}{e_i} \right|, \quad (22)$$

where  $e$  is a real value of a variable,  $\hat{e}$  is its estimate and  $n$  is the number of testings. A criteria for accepting a model as *proper* is that the model has a  $MMRE \leq 0.10$ .

The  $PRED(l)$  is defined as the quotient of number of cases in which the estimates are within the  $l$  absolute limit of the actual value divided by the total number of testings. It is considering a model is acceptable is  $PRED(0.1) \geq 0.9$ . This means that at least 90% of the estimates are within the range of the 10% of the actual values.

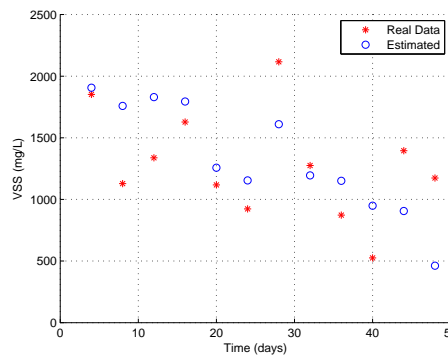
## 5.1 Case 1: State variables estimate

In this case the observer model designed estimates the organic substrate concentration ( $S_1$ ) and the acidogenic bacteria concentration ( $X_1$ ) and methanogenic bacteria concentration ( $X_2$ ) from measurable volatile fatty acids concentration ( $S_2$ ), assuming that the maximum acidogenic growth rate ( $\mu_{1max}$ ) and the maximum methanogenic growth rate ( $\mu_0$ ), are known and have a punctual and constant values (1.07 and 0.87, respectively).

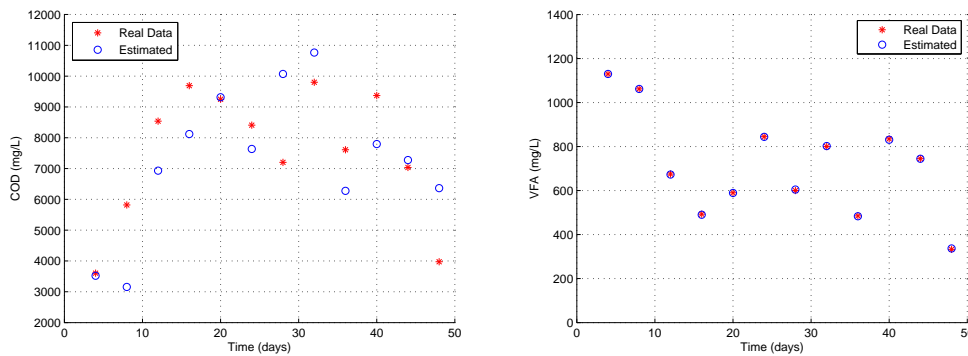
Figures 5 and 6 show results obtained at different operational conditions. Figure 5 shows comparison between volatile suspended solids (VSS) measurements and estimated values of acidogenic bacteria ( $X_1$ ) and methanogenic bacteria ( $X_2$ ) concentration. Figure 6 shows comparison between estimate values and measurements for organic substrate concentration expressed in terms of chemical oxygen demand (COD) and volatile fatty acids concentration (VFA).

Results obtained from the high-gain observer designed assuming the maximum growth rates punctual and constants (Case 1a) exhibit in general a MMRE of 0.8515 and PRED of 0.6666. That means that the criteria is not compliance because the MMRE is greater than 0.1 and only 67 % of the estimates are within the range of the 10 % of the real values. In Table 3 are presented the specific MMRE and PRED of each variable estimates. Is important to note that the estimated amount of volatile suspended solids concentration (VSS) present a large deviation with respect to the real values. Only 8% of the VSS estimates satisfy the criteria of  $PRED(0.1)$ .

The results does not exhibit the expected performance. It is proposed to use a set of maximum growth rate values to acidogenic stage to improve performance (Case 1b). The values of the set are presented in Table 4 and outcome are showing in Figures 7 and 8. Figure 7 shows the result of estimated values of acidogenic bacteria ( $X_1$ ) and methanogenic bacteria ( $X_2$ ) concentration



**Figure 5:** Comparison between VSS real data and estimated total biomass ( $X_1+X_2$ ) from measurable volatile fatty acids concentration assuming punctual values of maximum growth rates



**Figure 6:** Estimated values and measurements for COD and VFA, assuming punctual values of maximum growth rates

**Table 3:** Performance exhibit of the proposed observer models

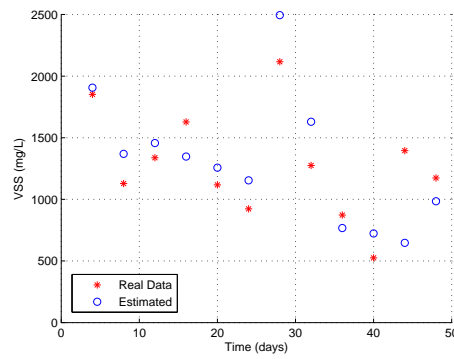
		Case 1a	Case 1b	Case 2
<b>Dataset 1: VSS</b>	MMRE	2.4885	0.2068	0.0311
	PRED(0.1)	0.0833	0.3333	1.0000
<b>Dataset 2: COD</b>	MMRE	0.0375	0.0770	0.0575
	PRED(0.1)	0.9167	0.8333	0.8333
<b>Dataset 3: VFA</b>	MMRE	0.0283	0.0010	0.0000
	PRED(0.1)	1.0000	1.0000	1.0000
<b>General</b>	MMRE	0.8515	0.0950	0.0952
	PRED(0.1)	0.6666	0.7222	0.9444

**Table 4:** Maximum acidogenic growth rate values set

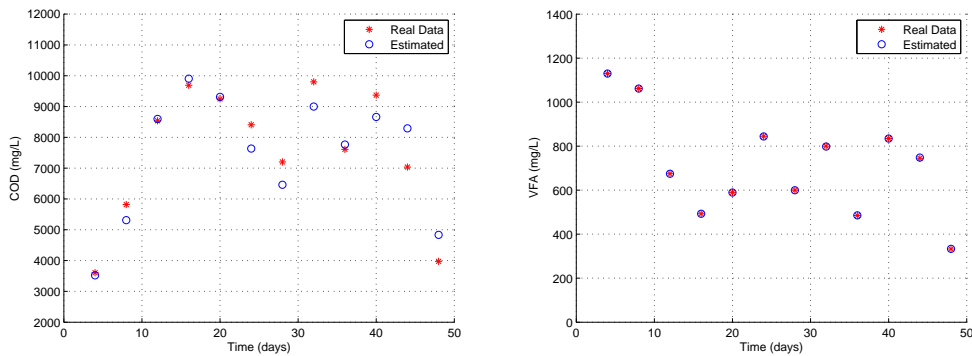
Organic substrate concentration, $S_{1in}$	Maximum acidogenic growth rate, $\mu_{1max}$
$\leq 8999$	2.00
9000 – 10999	0.61
11000 – 13999	1.07
14000 – 14999	0.85
15000 – 17999	1.34
$\geq 18000$	1.55

compared to volatile suspended solids (VSS) real data. Figure 8 shows the estimate values and measurements of organic substrate concentration expressed in terms of chemical oxygen demand (COD) and volatile fatty acids concentration (VFA).

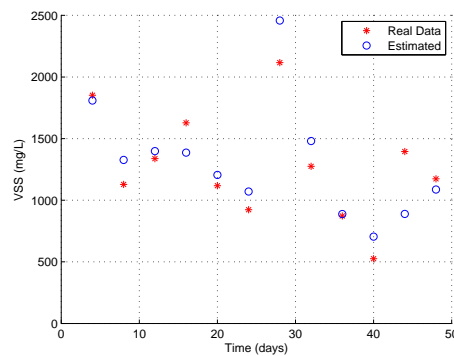
In general, the Case 1b presents a better performance to estimate the unknown variables and parameters using the set of maximum acidogenic rate values in the observer design. Is obtained a MMRE of 0.0950 and PRED of 0.7222, that means that the first criteria is met ( $MMRE \leq 0.10$ ) but only 72 % of the estimates are within the range of the 10 %. Although better performance is observed with respect to the model Case 1a. However, the estimating of the VSS does not met with the criteria of MMRE and PRED (See Table 3, Dataset 1, Case1b).



**Figure 7:** Comparison between VSS real data and estimated total biomass ( $X_1+X_2$ ) from measurable volatile fatty acids concentration



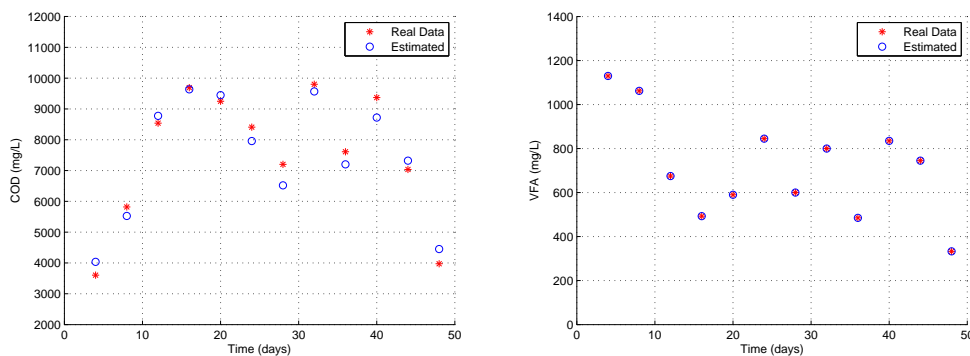
**Figure 8:** Estimate values and measurements for COD and VFA



**Figure 9:** Comparison between VSS data real and estimated total biomass ( $X_1+X_2$ ) from measurable volatile fatty acids concentration, assuming unknown parameters

## 5.2 Case 2: State variables and unknown parameters

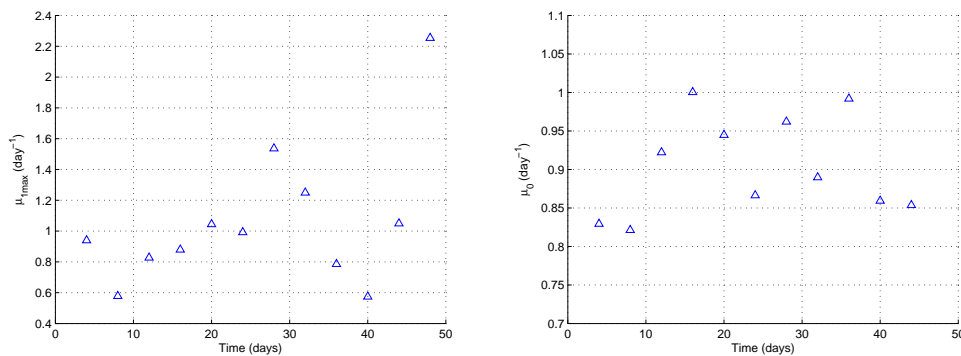
In this case it is assumed that the maximum acidogenic growth rate ( $\mu_{1max}$ ) and the maximum methanogenic growth rate ( $\mu_0$ ) are unknown and time-varying. The observer model estimates organic substrate concentration ( $S_1$ ), acidogenic bacteria concentration ( $X_1$ ), methanogenic bac-



**Figure 10:** Comparison between estimate values and measurements for COD and VFA, assuming unknown parameters

teria concentration ( $X_2$ ), and unknown parameters from volatile fatty acid concentration (VFA) measurement. Figures 9, 10 and 11 show the results obtained at different operational conditions. Comparison between volatile suspended solids (VSS) measurements and estimated values of acidogenic bacteria ( $X_1$ ) and methanogenic bacteria ( $X_2$ ) concentration is showed in Figure 9. Comparison between estimate values and measurements for organic substrate concentration ( $S_1$ ) expressed in terms of chemical oxygen demand (COD) and volatile fatty acids concentration (VFA), is showed in Figure. 10 and parameters values estimated are showed in Figure. 11.

The model designed presents an adequate performance to represent the dynamics of the system.



**Figure 11:** Estimated values of maximum acidogenic growth rate ( $\mu_{1max}$ ) and maximum methanogenic growth rate ( $\mu_0$ )

In general, the observer model to estimate state variables and unknown parameters presents a MMRE of 0.0952 and PRED of 0.9444. That means that the criteria is compliance due the MMRE is less than 0.1 and 94 % of the estimates are within the range of the 10 % of the real values. Table 3 shows the specific MMRE and PRED of each variable estimates. The VSS and VFA estimations meet the two criteria proposed (MMRE and PRED), nevertheless, the PRED(0.1) estimated in 0.83 of COD does not meet with the criteria of PRED(0.1)  $\geq 0.90$ .

## 6 Conclusions

This work is a preliminary study to propose a nonlinear observer model using adaptive high gain observers based on a phenomenological model of anaerobic digestion industrial process. Under normal conditions, anaerobic waste treatment proceeds with a minimum control [27]. However, if load disturbances occur or environmental conditions are suddenly changed, the process become unbalanced. Many parameters should be monitored for proper control of the process [38], however, the volatile acids concentration is one of the most important control test for anaerobic digestion.

The design of two observers is presented, the first observer is designed to estimate state variables and the second to estimate state variables and time-varying parameters unknown. In both cases, the measurable variable corresponds to volatile fatty acid concentration, which is an intermediate product of the anaerobic digestion reactor and its accumulation produce pH decrease, generating instability in the reactor until a possible washout.

In order to evaluate the performance of models designed the criteria used is to compute the values for  $MMRE \leq 0.1$  and  $PRED(0.1) \geq 0.90$ . Generally, the standard criteria for considering a model as acceptable are  $MMRE \leq 0.25$  and  $PRED(0.25) \geq 0.75$ , but in this study is necessary a higher precision and accuracy due to the processes requirements and uncertainty attached to the measurement of the real values.

In first case, during the design of the model was necessary include a set of maximum acidogenic growth rate values to obtain a better performance because the results of  $PRED(0.1)$  criteria value is not within the specified range. Then, the model designed only complies with the  $MMRE$  criteria, therefore it is necessary to implement a new assumptions. The second case presents a design of a nonlinear observers model assuming that the parameters are unknown. This model calculates organic substrate concentration, concentration of bacteria and the maximum growth rates. The model is considered as acceptable due it satisfies two specific criteria. The performance of the observer model designed in the second case is better than the first model to represent the dynamic of the anaerobic digestion processes.

The model proposed in this work and the associated methodology could be used for nonlinear control schemes design, since it takes into account modelling errors, parametric uncertainties and unmeasured disturbances.



## Nomenclature

$\text{CO}_2$	carbon dioxide concentration (mg/L)
$\text{CH}_4$	methane concentration (mg/L)
H	hydrogen concentration (mg/L)
D	dilution rate ( $\text{day}^{-1}$ )
$k_1$	yield for substrate degradation (mg $\text{S}_1$ /mg $\text{X}_1$ )
$k_2$	yield for VFA production (mg VFA/mg $\text{X}_1$ )
$k_3$	yield for VFA consumption (mg VFA /mg $\text{X}_2$ )
$K_{S1}$	half-saturation constant associated with $\text{S}_1$ (mg/L)
$K_{S2}$	half-saturation constant associated with $\text{S}_2$ (mg/L)
$K_I$	inhibition constant associated with $\text{S}_2$ (mg/L)
$k_d$	biomass decay rate ( $\text{day}^{-1}$ )
pH	potential of hydrogen
T	temperature ( $^{\circ}\text{C}$ )
$\text{S}_1, \text{S}_{1in}$	organic substrate concentration (mg/L)
$\text{S}_2, \text{S}_{2in}$	volatile fatty acids concentration (mg/L)
$\text{X}_1, \text{X}_{1in}$	concentration of acidogenic bacteria (mg/L)
$\text{X}_2, \text{X}_{2in}$	concentration of methanogenic bacteria (mg/L)
$t$	time (day)

### Greek letters

$\alpha$	proportion of dilution rate for bacteria (mg /L)
$\mu_{1max}$	maximum acidogenic biomass growth rate ( $\text{day}^{-1}$ )
$\mu_0$	maximum methanogenic biomass growth rate ( $\text{day}^{-1}$ )
$\Theta$	temperature activity coefficient
$\theta$	high gain

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