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State Estimation by Artificial Neural Networks in a Continuous Bioreactor

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Abstract: A based neural networks state observer to estimate biomass, substrate and methane in a continuous anaerobic reactor is introduced in this paper. The observer is designed from a recurrent high order neural network with a hyperbolic tangent as activation function and an extended Kalman filter as learning algorithm. The observer structure is validated via simulations and using experimental data obtained from an anaerobic continuous stirred tank at lab scale. This prototype is used to treat real slaughterhouse wastewater and it is operated in continuous mode. The obtained results show that the proposed observer is able to reproduce adequately the biomethane production and the substrate (related to chemical oxygen demand) in the methanogenesis stage; besides, methanogenic bacteria are also well estimated but some modifications are required in order to reach better results.

Keywords: neural observer; state estimation, anaerobic digestion; wastewater treatment; biogas.

1. INTRODUCTION

Wastes generation is directly related to the human activities. Most of industrial processes are based on the transformation of raw materials producing a large quantity of wastes. If they are not well managed, wastes can induce sever damages on the ecosystems and on the human health. A particular case is slaughterhouses; the animals sacrifice requires a large volume of water and produces different kinds of wastes: fat, blood, sludge, bones, and wastewater. Nowadays, some wastes are used to synthesize other products or reused in some applications; but in many cases, a lot of them are directly rejected to the ecosystem without an adequate treatment process (Mittal, 2006; Arvanitoyannis and Ladas, 2008). Concerning the use of water, according with the Food and Agriculture Organization (Quiroga Tapias and García de Siles, 1994), the processing of cattle and pigs requires 1000 L and 450 L of water per animal, respectively; it is considered that 95% of the water becomes wastewater and the other 5% is evaporated (Signorini, 2007). Then, it is important to implement efficient wastewater treatment processes in order to avoid environmental risks.

It is well known that biological processes offer important benefits in wastewater treatment. Specifically, anaerobic processes are well situated to treat effluents with high organic load: the complex organic molecules are progressively degraded in four successive stages (hydrolysis, acidogenesis, acetogenesis and methanogenesis) into a biogas mainly composed of methane and carbon dioxide (McCarty, 1964a, 1964b; Salminen and Rintala, 2002); then, this biogas can be used as an alternative source of energy. Each stage is developed by a different bacteria population forming a specific product which is used as input for next one. If the micro-organisms cannot transform the corresponding components, the subsequent stage is inhibited because there is not substrate to the bacterial growth; this situation occurs typically in hydrolysis and acidogenesis. Besides, the methanogenic bacteria have the slowest growth rate and then an eventual exceeding of substrate can block methanogenesis stage affecting the methane production and the organic wastes transformation. For this reason, methanogenesis is considered as the limiting step and it requires special attention (Parkin and Owen, 1986; Moletta et al., 1986). Moreover, this bioprocess is sensitive to variations on the operating conditions, such as pH, temperature, overloads, etc.

Supervision systems are essential tools in order to detect eventual dysfunctional behaviours on the process development. In this context, some important variables which are necessary for supervision and control of anaerobic digestion are hard to measure or immeasurable. For example, biomass behaviour and chemical oxygen demand (COD) are good indicators of the biological activity inside the reactor. However, biomass sensors are quite expensive and they are not necessarily designed from an automatic control perspective, and then, it is difficult to apply those sensors on control systems. Besides, COD measurement is done off-line from laboratory analysis which requires more than two hours; this delay could affect the reactor performances and could induce some problems on the process operation, especially in the case of overloads or changes on the operating conditions. Observers and softsensors are an interesting alternative in order to overcome this situation.

Different observers have been already reported, such as the asymptotical observer, proposed by Bastin and Dochain (1990), interval observers (Smith, 1996; Gouze, Rapaport and Hadj-Zadok, 2000, Alcaraz-Gonzalez et al. (2004)), and other approaches (Deza et al., 1993; Chachuat and Bernard, 2005).

Some of them are developed focusing on diagnosis and fault detection, such as Lardon, Punal and Steyer (2004), Wimberger & Verde (2008). Fuzzy algorithms have been also considered as alternatives to design observers and controllers for bioprocesses (Ascencio, Sbarbaro and Feyo de Azevedo, 2004, Carlos-Hernandez et al, 2009). Complete knowledge of the system model is usually assumed in order to design nonlinear state estimators; nevertheless this is not always possible. Moreover, in some cases special nonlinear transformations are proposed, which are not often robust in presence of uncertainties. An interesting approach for avoiding the associated problem of model-based state observers is the neural networks approach. Neural observers require feasible measures and a training algorithm in order to learn the process dynamics; in this case, the model knowledge is not strictly necessary (Pozniak et al., 2001; Belmonte-Izquierdo et al., 2010; Gurubel et al., 2011).

In this paper, a Recurrent High Order Neural Observer (RHONO) is proposed in order to estimate biomass, substrate and biogas in an anaerobic process for slaughterhouse effluents treatment. The observation scheme considers a hyperbolic tangent as activation function and an extended Kalman filter as learning algorithm. The observer is validated in a lab scale process which uses real slaughterhouse wastewater and it is operated in continuous mode. An important advantage of this observer is the high performance and independence of the process model.

2. MATERIALS AND METHODS

2.1 Lab scale process description

The experimental set up considered in this work is based on an anaerobic reactor continuously stirred and it is operated in continuous mode. Fig. 1 illustrates this process.

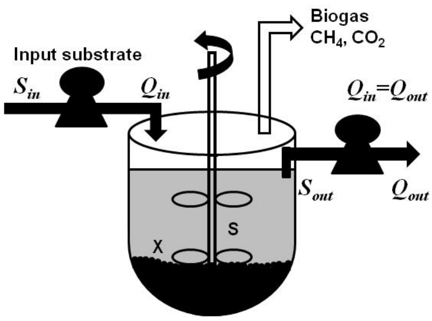

Fig. 1. Anaerobic reactor with immobilized bacteria.

where S, S_{in} and S_{out} represent substrate as the reaction medium, input substrate and treated medium respectively; X is the biomass, Q_{in} the input flow rate, Q_{out} the output flow rate and CH_4 and CO_2 are methane and carbon dioxide.

The volume of the glass reactor is 7 L and the prototype is equipped with sensors of pH, Temperature, revolutions per minute and volume level; the measurements of these parameters are collected by a data acquisition system. In addition, the produced biogas is measured by liquid displacement in a graduated column and the biogas composition is analyzed by gas chromatography. The reactor is stirred at 150 rpm in order to allow the reaction volume to be homogeneous and to keep bacteria fixed on the solid support. The input and output flow rates are controlled by independent pumps in order to guarantee the same flow rate in the influent and the effluent, and then a constant volume inside the reactor.

It is worth to mention that, anaerobic bacteria are fixed in a natural zeolite since previous results show the potential of this material to be used as support for anaerobic bacteria (Diaz-Jimenez et al., 2008).

2.2 Experimental methodology

The experiments were performed in two operating modes: batch and continuous. On batch mode, input and output flow rates are equal to zero; bacteria and substrate stay inside the reactor without external manipulation; the experiment is over when most of the substrate is transformed and no more biogas production is detected. In this work, the batch experiments are used for biomass adaptation to the substrate and are performed as follows: 4.5 L of wastewater and 500 mL of zeolite colonized by anaerobic bacteria are filled in the reactor at T=37°C. The wastewater is used directly from the slaughterhouse without dilution, then, the COD is ranged between 4500 to 9000 mg/L depending on the slaughterhouse operating conditions. If pH is very acid (around 5), it is adjusted around 7 adding a solution of sodium bicarbonate; if pH is alkaline no regulation is done. Batch tests are developed in 10-15 days duration according with the COD removing and biogas production. Concerning the continuous mode, the volume inside the reactor is constant; then the input and output flow rates are equal and the influents are treated continuously. Besides, the operating conditions can be modified (the substrate pH, the COD, the input flow rate) if required. The continuous mode is considered in this study to validate the proposed neural observer. The experiments are performed as follows: first, a batch experiment is performed in order to reach the steady state; at the end of this batch experiment the initial conditions for a continuous experiment are reached. After that, the input and output flow rates are activated. Considering the reaction volume, a low flow rate is selected in continuous operation: Q_{in}=Q_{out}=0.4 L/h. At the beginning of continuous regime, it is recommended to supervise carefully the biological activity through pH and biogas production; the acidity could increase due to the input substrate and to the production of acids on acidogenesis stage; after that the biological activity leads to steady state because of the bacteria adaptation to the operating conditions. At this moment, the input COD can be modified.

2.3 Neural observer structure

The use of multilayer neural networks is well known for pattern recognition and for modelling of static systems; the NN is usually trained to learn an input-output mapping. For control tasks such as state observers design, some extensions of the first order Hopfield model have been proposed in order to include more interactions among the neurons. An example of these extensions is the so called Recurrent High Order Neural Networks (RHONN). The RHONN are very flexible and allows incorporating into the neural model priory information about the system structure. Besides, discrete-time neural networks are better fitted for real-time implementations (Gurubel et al., 2011).

Let consider a discretized nonlinear system represented by:

$$x_{k+1} = F(x_k, u_k) + d_k \qquad (1)$$
$$y_k = h(x_k)$$

where k is a real number representing a time sample, $x \in R^n$ is the state vector of the system, $u \in R^m$ is the input vector, $y \in R_p$ is the output vector, $h(x_k)$ is a nonlinear function of the system states, $d_k \in R^n$ is a disturbance vector, F(•) is a smooth vector field; hence, the components of (1) can expressed as:

$$\begin{aligned} x_k &= [x_{1,k} \dots x_{i,k} \dots x_{n,k}]^T, \\ d_k &= [d_{1,k} \dots d_{i,k} \dots d_{n,k}]^T, \\ x_{i,k+1} &= F_i(x_k, u_k) + d_{i,k}, \qquad i = 1,\dots, n, \\ y_k &= h(x_k). \end{aligned} \qquad (2)$$

A neural observer for previous system can be implemented having the form of equations (3):

$$\begin{aligned} \hat{x}_k &= [\hat{x}_{1,k} \dots \hat{x}_{i,k} \dots \hat{x}_{n,k}]^T, \\ \hat{x}_{i,k+1} &= w_i^T z_i(\hat{x}_k, u_k) + g_i e_k, \\ \hat{y}_k &= h(\hat{x}_k); \qquad i = 1,\dots, n, \end{aligned} \qquad (3)$$

with $g_i \in R^p$ a like-Luenberger observer gain, u_i the external input vector to the NN and z_i a function of states and inputs to each neuron (Sanchez et al., 2008):

$$z = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_L \end{bmatrix} = \begin{bmatrix} \prod_{j \in I_1} y_j^{d_j(1)} \\ \prod_{j \in I_2} y_j^{d_j(2)} \\ \vdots \\ \prod_{j \in I_L} y_j^{d_j(L)} \end{bmatrix} \qquad (4)$$

The extended Kalman Filter is used as training algorithm; the main objective is to update on-line the weight vectors w_i. This algorithm is resumed below and more details can be found in (Sanchez et al., 2008):

$$\begin{aligned} w_{i,k+1} &= w_{i,k} + \eta_i K_{i,k} e_{i,k}, \\ K_{i,k} &= P_{i,k} H_{i,k} M_{i,k}, \\ P_{i,k+1} &= P_{i,k} - K_{i,k} H_{i,k}^T P_{i,k} + Q_{i,k}, \end{aligned} \qquad (5)$$

$$\begin{aligned} &with: \\ M_{i,k} &= [R_{i,k} + H_{i,k}^T P_{i,k} H_{i,k}]^{-1} \\ e_{i,k} &= y_k - \hat{y}_k, \end{aligned} \qquad (6)$$

where $e_{i,k} \in R^P$ is the observation error, $P_{i,k} \in R^{LixLi}$ is the prediction error covariance matrix at step k, $w_{i,k} \in R^{Li}$ is the weight (state) vector, L_i is the respective number of neural network weights, $y \in R^P$ is the plant output, y is the NN output, η_i is the learning rate, $K_{i,k} \in R^{LixP}$ is the Kalman gain matrix, $Q_{i,k} \in R^{LixLi}$ is the NN weight estimation noise covariance matrix, $R_{i,k} \in R^{PxP}$ is the error noise covariance, and $H_{i,k} \in R^{LixP}$ is the matrix for which each entry (H_{ij}) is the derivative of the *i-th* neural output with respect to *ij-th* NN weight, (w_{ij}). Where $i = 1,\dots, n$ and $j = 1,\dots, L_i$.

The structure of the proposed neural observer scheme is shown in Fig. 2.

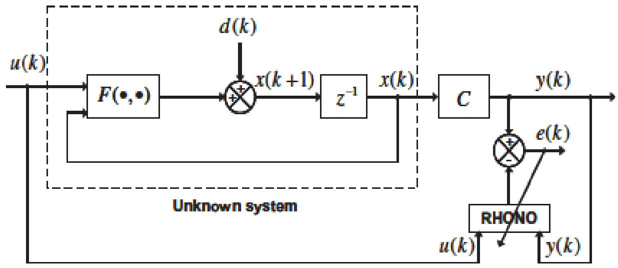

Fig. 2. Structure of the neural observer.

where the inputs (u) are dilution rate, input substrate and input inorganic carbon; the outputs (y) are methane and carbon dioxide. The states to be estimated are biomass, substrate and inorganic carbon.

3. OBSERVER DEVELOPMENT

3.1 Design

The mathematical representation of the neural observer is introduced by equations (7). It is based on the structure of a general model of anaerobic processes; linear, quadratic and more complex terms can be used in order to allow the NN to learn the different dynamics of each variable. In this case, three variables are considered in this work: methanogenic biomass, COD (represented by S) and Inorganic carbon.

$$\begin{aligned} \hat{X}(k+1) &= w_{11}\zeta(\hat{X}(k)) + w_{12}\zeta(\hat{X}(k))^2 + w_{13}D_{in}(k)\zeta(\hat{X}(k))^2 + g_1 e(k) \\ \hat{S}(k+1) &= w_{21}\zeta(\hat{S}(k)) + w_{22}\zeta(\hat{S}(k))S_{in}(k) + w_{23}D_{in}(k)\zeta(\hat{S}(k)) + g_2 e(k) \\ I\hat{C}(k+1) &= w_{31}\zeta(I\hat{C}(k)) + w_{32}\zeta(\hat{S}(k))D_{in}(k) + w_{33}\zeta(\hat{S}(k))IC_{in} + g_3 e(k) \end{aligned} \qquad (7)$$

Depending on the NN application, the activation function, ζ(•), can be chosen from different alternatives, e.g. threshold, piecewise-linear, sigmoid (logistic function, hyperbolic tangent function), radial base. As shown in (8), in this work, the hyperbolic tangent is used since the antisimetric functions allow the neural network to learn the process dynamic faster than other activation functions (Sanchez et al., 2008).

$$\begin{aligned} \zeta(\hat{X}(k)) &= \alpha_1 \tanh(\beta_1 \hat{X}(k)) \\ \zeta(S(k)) &= \alpha_2 \tanh(\beta_2 \hat{S}(k)) \\ \zeta(I\hat{C}(k)) &= \alpha_3 \tanh(\beta_3 I\hat{C}(k)) \end{aligned} \qquad (8)$$

The process outputs are given by the gaseous phase of anaerobic digestion. Methane and carbon dioxide are considered as in equations (9):

$$\hat{Q}_{CH4} = \gamma_1 f_{CH4}(\hat{X}(k)) \\ \hat{Q}_{CO2} = \gamma_2 f_{CH4}(\hat{X}(k)) \tag{9}$$

where γ_1 and γ_2 are production yields, which are determined from experimental data. Besides, f_{CH4} and f_{CO2} are functions describing the production of biogas, their structure is based on the traditional anaerobic processes.

3.2 Tuning guidelines

Tuning of the observer parameters could be difficult; some basic guidelines are provided in this section; more details can be found in (Sanchez et al., 2008; Belmonte-Izquierdo et al., 2010):

a). The covariance matrices for the EKF are initialized as diagonal matrices, they should verify the next condition:

$$P_i(0) > R_i(0) > Q_i(0) \tag{10}$$

It implies that *a priori* knowledge is not required to initialize the vector weights. In fact, higher entries in $P_i(0)$ correspond to a higher uncertainty in the *a priori* knowledge. It is advisable to set $P_i(0)$ inside the range 100-1000, and so on for the other covariance matrices on (10). The variation of those matrices has an effect on the efficiency to learn different dynamics of the process. For the observer described in this paper, the matrices are initialized as follows:

$$P_1(0) = P_2(0) = P_3(0) = 1000 \\ R_1(0) = R_2(0) = R_3(0) = 1 \\ Q_1(0) = Q_2(0) = Q_3(0) = 0.1 \tag{11}$$

An arbitrary scaling can be applied to $P_i(0)$, $R_i(0)$, and $Q_i(0)$ without altering the evolution of the weight vector.

b). Since the neural network outputs do not depend directly on the weight vector, the matrix H is initialized as $H_i(0)=0$.

c). It is assumed that weights values are initialized to small random values with zero mean value and normal distribution.

d). The learning rate determines the magnitude of the correction term applied to each neuron weight; it usually requires small values to achieve good training performance. Then, it is bounded as $0 < \eta < 1$.

e). The observer gain (g) is set by trial and error. It is bounded as $0 < L < 1$ for a good performance on the basis of training experience.

f). Coefficients α and β in equations (8) are obtained from simulations. These coefficients have an influence on the respective variable estimation; then it is important to find a compromise concerning the estimation of all the considered variables. The set of values which provide the better results were: $\alpha_1 = \alpha_2 = \alpha_3 = 1$ and $\beta_1 = \beta_2 = 1$; $\beta_3 = 110$.

4. RESULTS

First, a series of simulations is developed in order to evaluate the observer performances; a model previously validated has been used as reference data (Belmonte-Izquierdo et al., 2010). The obtained results are shown in Fig. 3 to Fig. 5. The observer has been initialized randomly in order to test the observer convergence, which is illustrated at the beginning of the simulation: the estimated state reach the model one in few minutes. After the convergence, the estimation is done with high quality; the error estimation is negligible for the three variables. In addition, a variation on the input substrate is simulated: an increase of 100% of the initial condition is considered from t = 300 h to t = 600h. The three variables are well estimated despite this change on the operating conditions, which means the observer is able to follow the process dynamics in face of input disturbances.

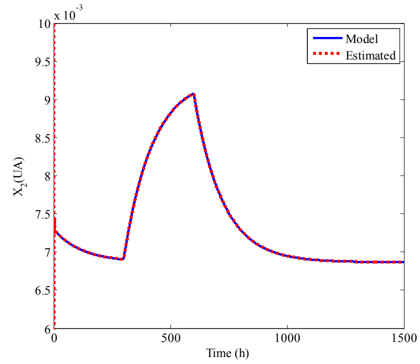

Fig 3. Biomass estimation.

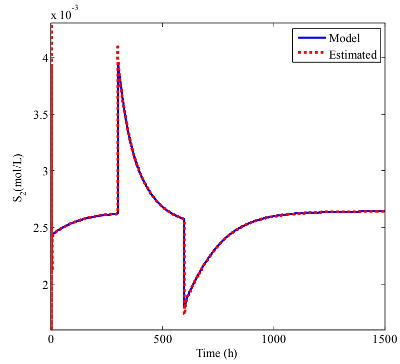

Fig. 4. Substrate estimation.

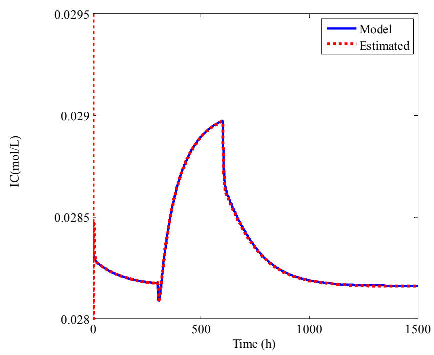

Fig. 5. Inorganic Carbon estimation.

After that, the observer is tested using experimental data. The input substrate is equivalent to the measured COD in the effluent provided by the slaughterhouse; as said before, the samples are used directly without any additional modification. The input flow rate was Q_{in} = 0.45 L/h. The input substrate considered in the experiment is presented in Fig. 6.

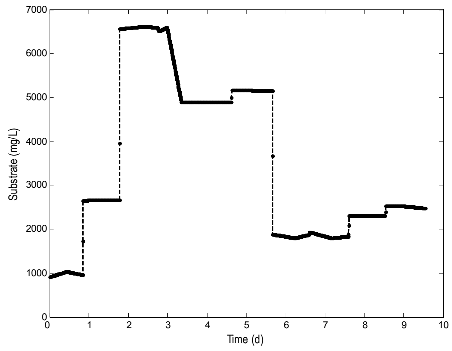

Fig. 6. Input substrate

The biomass estimation is presented in Fig. 7. As can be remarked, the observer has some problems to recover the biomass behaviour. A possible reason is that the training data do not contain the complete dynamics of bacteria; also, the structure of the neural observer is simple and maybe it is required to add some other neurons, especially for the section concerning biomass; for example, it is likely necessary to include a relationship between methane and biomass since the presented structure does not consider it.

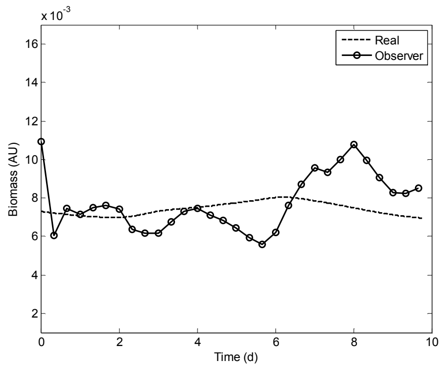

Fig 7. Real biomass estimation

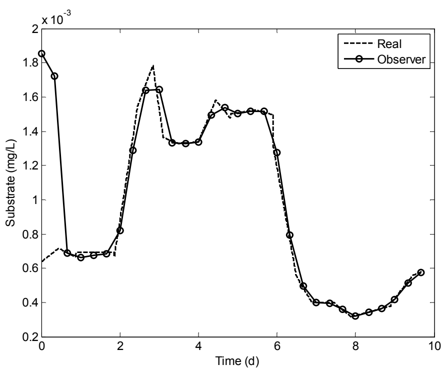

Fig. 8. Real substrate estimation

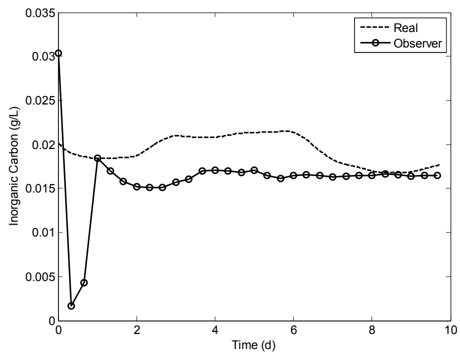

Fig. 9. Real inorganic carbon estimation

On the other side, substrate and inorganic carbon are well estimated by the neural observer as can be seen in Fig. 8 and Fig. 9, respectively. At the beginning of the experimentation, the convergence is illustrated: the observer is initialized randomly and after 10 h, approximately, it meets the real variable. After the convergence, the estimation is done almost perfectly for the substrate and with a small estimation error for the inorganic carbon. The dynamics of inorganic carbon is faster than the substrate, it is a possible reason of the estimation error; as for the biomass, other neurons should be added to the neural structure in order to improve the estimation of this variable. Besides, the use of variable parameters and a self-tuning methodology could allow the neural network to better adapt their learning capability of complex dynamics and then to improve the estimation.

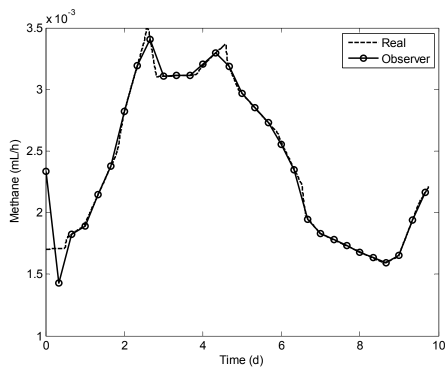

Fig. 10. Real methane estimation

Concerning the methane estimation, the results are presented in Fig. 10. After the convergence, the estimation is done with a negligible error; this is an expected situation since the measures of methane are used for the estimation. However, it is worth to mention that the estimation is adequate in all the experimentation time, even for the cases where no measures are provided. This is in an important advantage of the observer since methane is a good indicator of the biological activity and it is very useful for supervision purposes; the existing biomethane sensors are expensive and then the neural observer is an interesting alternative. In addition, in previous works a similar structure has been tested by using a synthetic substrate (Belmonte-Izquierdo et al., 2010); the application for more complex substrate, such as the ones from slaughterhouse considered here, proves the flexibility of the neural observer related to the kind of substrates.

5. CONCLUSIONS

A neural observer has been proposed in this paper. The main objective was to estimate biomass, substrate and biomethane in anaerobic process; additionally, estimation of inorganic carbon is also included in the structure of the observer. The observer is validated via simulations and by experimental data obtained from a continuous bioreactor treating real slaughterhouse wastewater. The obtained results show a well estimation of substrate, inorganic carbon and biomethane. Biomass is estimated with errors, but it can be said that the behaviour is reproduced qualitatively. The observer structure was selected simple in order to reach a compromise between complexity for real implementation and estimation quality.

Current works are in progress in order to improve the observer performances, especially for biomass which is an important variable in anaerobic processes. The idea is to include more neurons in the observer structure, to enhance the tuning methodology, and also to use some other data to train the neural network.

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