

ON-LINE ESTIMATION OF UNMEASURED INPUTS FOR ANAEROBIC PROCESS DESCRIBED BY INTERPOLATED L.T.I. MODELS.

D. Theilliol^(*), C. Aubrun^(*), J-C Ponsart^(*) and J. Harmand^(**)

^(*) Centre de Recherche en Automatique de Nancy - CNRS UMR 7039
BP 239 - 54506 Vandoeuvre Cedex - France.

^(**) Laboratoire de Biotechnologie de l'Environnement - INRA
Avenue des Etangs - 11100 Narbonne - France.

email: didier.theilliol@cran.uhp-nancy.fr
Phone: +33 383 912 701 - Fax: +33 383 912 030

Abstract: A method for unknown input estimation in nonlinear stochastic system is presented. A key problem in bioprocess systems is the absence, in some cases, of reliable on line measurements for real time monitoring applications. In this paper, a software sensor for an anaerobic digester is presented. Unmeasured components of the influent are estimated from available on line measurements. Based on a multiple model scheme, a bank of unknown input Kalman filters are discussed to estimate a probabilistic weighting state and unknown input of the process. The performances of the method are tested in simulation using a validated model of an anaerobic fixed bed pilot plant.
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Keywords: Interpolated L.T.I. models, unknown inputs, Kalman filter, multiple model algorithm, nonlinear systems, biological process.

1. INTRODUCTION

One of the most frequent and important challenges in the control of chemical and biochemical processes is to find adequate and reliable sensors to measure key variables of the plant. However, if a number of sensors providing direct real time measurements of the state variables are today available at the industrial scale, they are still very expensive and their maintenance is usually time consuming, especially in the field of chemical and biological processes. Furthermore, biological processes are highly nonlinear systems and their kinetic parameters are usually badly or poorly known. To overcome these difficulties, the notion of *software sensors* has been introduced. In fact, these software sensors consist in using state estimation techniques to reconstruct time evolution of the unmeasured states from the available on-line measurements. Besides the extended Kalman filter, several approaches have been proposed since the early eighties. Some approaches are based on linearization methods (Nicosia *et al.*, 1986). Other approaches are sliding observers based on the theory of variable structure systems, (Walcott and Zak, 1986) or based on the set theoretic approach for linear systems where the unknown nonlinearities are considered either as bounded (Misawa and Hedrick,

1989), or as system perturbations (Hou and Muller, 1994). These methods have been successfully applied to biological and chemical processes (Bastin and Dochain, 1990; Farza *et al.*, 1998). In the stochastic case, some results have been obtained for optimal unknown input decoupling purpose (Aubrun *et al.*, 2001) around an operating point. This paper is concerned with the design and application on an anaerobic digester of a bank of Kalman filters for software sensor purpose. The process is represented by an interpolated discrete linear time invariant model obtained from mass balance equations of the anaerobic digester.

The paper is organised as follows. Section 2 presents a general theory and the design procedure to estimate the unmeasured input applied to a nonlinear system described by a set of interpolated linear time invariant models. The section 3 is devoted to the dynamical model development of the considered anaerobic wastewater treatment process. In the next section, the simulation results of the considered process are then shown and commented. Based on the nonlinear model of the system and the simulation measurements, the unknown inputs are estimated in a wide range of variations. Finally, concluding remarks are given.

2. UNMEASURED INPUTS ESTIMATION

Consider a discrete nonlinear system described by the following discrete state space representation:

$$\begin{aligned} X(k+1) &= F(X(k), U(k), D(k)) + W(k) \\ Y(k) &= G(X(k)) + V(k) \end{aligned} \quad (1)$$

where $X \in \mathfrak{R}^n$ is the state space, $U \in \mathfrak{R}^p$ is the input vector, $D \in \mathfrak{R}^q$ is the unknown input vector; $Y \in \mathfrak{R}^m$ is the output vector; $W \in \mathfrak{R}^n$ (respectively $V \in \mathfrak{R}^m$) represents the plant noise vector (respectively the measurement noise vector), $F(\cdot)$ and $G(\cdot)$ are smooth nonlinear functions.

Let us assume that the nonlinear system (1) can be modeled as a set of linear systems around z operating points. Each operating point is defined by a couple of input-output measurements defined as: $(Y_{i0}, U_{i0}, X_{i0}, \forall i \in [1 \dots z])$. A linear stochastic state space representation is associated with each operating point described by the following form:

$$\begin{aligned} x_{k+1}^i &= A_i x_k^i + B_i u_k^i + H_i d_k^i + w_k^i \\ y_k^i &= C_i x_k^i + v_k^i \end{aligned} \quad (2)$$

where (A_i, B_i, C_i, H_i) are the system matrices, $x^i \in \mathfrak{R}^n$ is the state vector, $u^i \in \mathfrak{R}^p$ is the control input vector, $d^i \in \mathfrak{R}^q$ is the unknown input vector and $y^i \in \mathfrak{R}^m$ is the output vector around the i^{th} operating point. It is assumed that $\forall i, \text{rank}(C_i) = m$ and $\text{rank}(H_i) = q$. w^i and v^i are independent zero mean white noise sequences with covariance matrices Q_i and R_i around the i^{th} operating point ($\forall i \in [1 \dots z]$).

The dynamic of the system in exactly z operating points is known and span the entire range of operating zone of the nonlinear plant (Johansen et al., 1998).

Based on this assumption, model validity functions mvf_k^i can be used to evaluate the validity of each linear model such that:

$mvf_k^i \rightarrow 1$: when the i^{th} model satisfactorily describes the behavior of the non linear system

$mvf_k^i \rightarrow 0$: otherwise

with $\sum_{i=0}^z mvf_k^i = 1$ which implies that as the nonlinear

system moves onto an operating point where one of the z models becomes more trustworthy than the others, the other models lose their validity.

The probability for each of the assumed models is calculated as a function of the actual and estimated measurements. Then the model considered at sample k is determined as the conditional mean value among

all the set of z models. The maximum likelihood estimate is the value which has the highest probability. The implementation of the procedure is realised by means of a bank of Kalman linear filters.

This bank is used to estimate the state \hat{x}_k^i and outputs

\hat{y}_k^i and generate a residual vector $r_k^i = y_k^i - \hat{y}_k^i$ around the i^{th} operating point. The residuals of the considered filter, around the corresponding operating point, follow a Gaussian distribution. Then assuming stationarity property of the residual, the probability distribution function, noted pdf_k^i , is defined as:

$$pdf_k^i = \frac{\exp\left\{-0.5 \times r_k^i \times (\Omega_k^i)^{-1} \times r_k^{iT}\right\}}{\sqrt{2\pi \times \Omega_k^i}} \quad (3)$$

where Ω_k^i defines the covariance matrix of the residuals r_k^i .

Based on the probability distribution function, a mode probability, noted $proba_k^i$, can be calculated applying Bayes theorem $\forall i \in [1 \dots z]$ (Banerjee et al., 1995):

$$proba_{k+1}^i = \frac{pdf_k^i \times proba_k^i}{\sum_{h=1}^z pdf_k^h \times proba_k^h} \quad (4)$$

The model validity functions, mvf_k^i , are computed by using (eq 4). Therefore, the probability estimation algorithm can get locked onto one model so that the probability converges to one, while the one associated to the other models converges to zero. The mode probabilities, $proba_k^i$, are used to isolate the actual operating point.

Following the approach developed by (Maybeck, 1999), a non linear system can be approximated by a finite number of interpolated linear time invariant models through the generation of probabilistically weighted state estimate vector, \hat{X} ,

$$\hat{X}_k = \sum_{i=1}^z (proba_k^i \times \hat{x}_k^i) + \sum_{i=1}^z (proba_k^i \times X_{i0}) \quad (5)$$

The mode probability calculation is based on the residual generation. A classical estimation procedure is carried on for each of the z assumed linear time invariant models as:

$$\begin{aligned} \hat{x}_{k+1}^i &= A_i \hat{x}_k^i + B_i u_k^i + K_k^i (y_k^i - C_i \hat{x}_k^i) \\ \hat{y}_k^i &= C_i \hat{x}_k^i \end{aligned} \quad (6)$$

where \hat{x}^i and \hat{y}^i denote the state and output estimation vectors around the i^{th} operating point ($\forall i \in [1 \dots z]$). K^i represents the gain of the i^{th} Kalman filter.

From equations (2) and (6), the estimation error $e_k^i = (x_k^i - \hat{x}_k^i) \in \mathfrak{R}^n$ and the output residuals $r_k^i = (y_k^i - \hat{y}_k^i) \in \mathfrak{R}^m$ propagate as:

$$\begin{aligned} e_{k+1}^i &= (A_i - K_k^i C_i) e_k^i + H_i d_k^i - K_k^i v_k^i + w_k^i \\ r_k^i &= C_i e_k^i + v_k^i \end{aligned} \quad (7)$$

The output residuals are corrupted by effects of unknown inputs and are not zero-mean value although the i^{th} model exactly matches the non linear system. According to the operating regimes, the use of a model set in the estimation algorithm results in a poor performance in the presence of unknown inputs. In order to generate some residuals sensitive to operating points and insensitive to unknown inputs, considered as faulty inputs, a bank of full-order Kalman filter with unknown inputs is proposed (Keller, 1999). Compared to other approaches (Darouach *et al.*, 1995), the full-order Kalman filter generates an innovation insensitive to unknown inputs through a reduced output residual vector so that its j^{th} component is decoupled from all but the j^{th} unknown inputs.

Therefore, the proposed bank of filters provides state estimation and unknown inputs estimation. Based on the linear model, defined in (2), and under the assumption that $\forall i \in [1 \dots z], \text{rank}(C_i F_i) = q \leq m$, (that is to say that the unknown inputs are independent and the number of unknown inputs are less than the number of measured outputs), each filter is defined by the following relations:

$$\hat{x}_{k+1}^i = A_i \hat{x}_k^i + B_i u_k^i + \bar{K}_k^i \gamma_k^i + \omega_i \beta_k^i \quad (8)$$

$$\bar{K}_k^i = \bar{A}_i P_k^i \bar{C}_i^T \left(\bar{C}_i P_k^i \bar{C}_i^T + \bar{V}_i \right)^{-1} \quad (9)$$

$$\begin{aligned} P_{k+1}^i &= \left(\bar{A}_i - \bar{K}_k^i \bar{C}_i \right) P_k^i \left(\bar{A}_i - \bar{K}_k^i \bar{C}_i \right)^T \\ &\quad + \bar{K}_k^i \bar{V}_i \left(\bar{K}_k^i \right)^T + \bar{Q}_i \end{aligned} \quad (10)$$

with $\bar{A}_i = (A_i - \omega_i \Pi_i C_i)$, $\bar{C}_i = \Sigma_i C_i$, $\bar{V}_i = \Sigma_i R_i \Sigma_i^T$, and $\bar{Q}_i = Q_i + \omega_i \Pi_i R_i \Pi_i^T \omega_i^T$.

where $\Pi_i = (C_i H_i)^+$, $\omega_i = A_i H_i$ and $\Sigma_i = \alpha_i (I_m - C_i H_i \Pi_i)$. $\alpha_i \in \mathfrak{R}^{m-q \times m}$ is an arbitrary matrix determined so that matrix Σ_i is of full rows rank.

Following those assumptions, γ_k^i and β_k^i are given by $\gamma_k^i = \Sigma_i (y_k^i - C_i \hat{x}_k^i)$ and $\beta_k^i = \Pi_i (y_k^i - C_i \hat{x}_k^i)$. γ_k^i and β_k^i have the following properties:

$\gamma_k^i \in \mathfrak{R}^{m-q}$ is decoupled from the unknown inputs.

$\beta_k^i \in \mathfrak{R}^q$ represents an estimation of the magnitudes of the unknown inputs d_k^i .

Therefore the new residuals vector γ_k^i , insensitive to unknown inputs and followed a Gaussian distribution, can be substituted into equation (3) to obtain an i^{th} mode probability close to one when the i^{th} model describes the behaviour of the non linear system in spite of the unknown inputs effects.

Moreover, an accurate state and unknown inputs accurate estimation are generated according to probabilistically weighted principle given as:

$$\hat{X}_k = \sum_{i=1}^z \left(\text{proba}_k^i \times \hat{x}_k^i \right) + \sum_{i=1}^z \left(\text{proba}_k^i \times X_{i0} \right) \quad (11)$$

$$\hat{D}_k = \sum_{i=1}^z \left(\text{proba}_k^i \times \hat{d}_k^i \right) + \sum_{i=1}^z \left(\text{proba}_k^i \times D_{i0} \right) \quad (12)$$

Under the assumption that the actual non linear system does not switch to one linear model to another at every sampling periods, the stability and the convergence of the unknown input Kalman filter depend on the properties of each decoupling filter. Necessary and sufficient conditions for stability and convergence of each filter are established in (Keller, 1999).

4. APPLICATION RESULTS

4.1 Process description.

The process under interest in this study is a 948 litter fixed bed anaerobic pilot plant used for the treatment of wine vinasses. The reactor is a circular column of 3.5 m in height, 0.6 m in diameter. A recirculation loop ensures the homogeneity of the liquid phase in the tank. The synoptic of the plant is represented in Fig. 1.

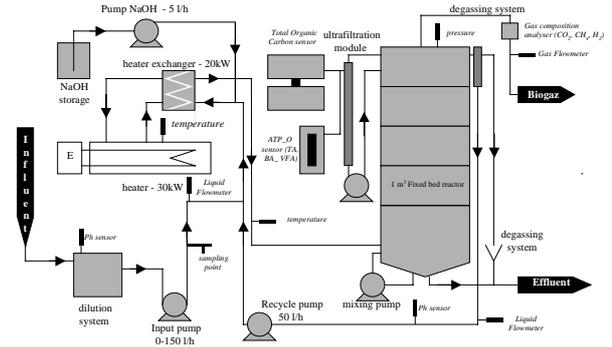


Fig. 1. Schematic representation of the plant

This process is located at the "Laboratoire de Biotechnologie de l'Environnement" (LBE), a lab from the french national institute for agronomic research (INRA) in Narbonne, France. It is automatically operated to validate new control or supervision algorithms. This highly instrumented process is equipped with a dilution system that allows the user to simulate input disturbances while the control action is the input flow rate. A constant 35°C temperature is maintained using a heat exchanger located in the recirculation loop.

The available instrumentation includes the measurement of gas flow rate and composition, partial CO₂ pressure. In addition, an on-line automatic titration sensor, called ATP_O and developed by LBE INRA in Narbonne is also connected to the ultra-filtration loop. It permits the acquisition of on-line partial and total alkalinity measurements every 3 minutes if required. It also gives on-line estimates of the bicarbonate and VFAs concentrations in the output of the reactor with a high

accuracy. An additional characteristic is that the maintenance requirements are totally compatible with industrial needs (only one manual operation per week). Last but not least, this sensor was proven to be very useful to achieve very good monitoring and control of the anaerobic digestion process (Bernard *et al.*, 2000). Finally the output COD (Chemical Organic Demand) is estimated from the measurement delivered by an industrial TOC (Total Organic Carbon) sensor. The input pH and the recirculation flow rate are locally controlled.

All these sensors are connected to an input/output device that allows the acquisition, treatment and storage of data on a PC using the Modular SPC[®] software. This software, also developed by LBE-INRA in Narbonne, performs advanced control law calculations as well as process supervision (Steyer *et al.*, 1997). In the following, a model of the considered anaerobic digestion process is given.

4.2 Nonlinear Model

The nonlinear mass balance model of the anaerobic digestion process is given by the following Ordinary Differential Equation system (Bernard *et al.*, 1998):

$$\begin{cases} \dot{X}_1 = (\mu_1 - \alpha D_r) X_1 \\ \dot{X}_2 = (\mu_2 - \alpha D_r) X_2 \\ \dot{Z} = D_r (Z^i - Z) \\ \dot{S}_1 = D_r (S_1^i - S_1) - k_1 \mu_1 X_1 \\ \dot{S}_2 = D_r (S_2^i - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \\ \dot{C}_{TI} = D_r (C_{TI}^i - C_{TI}) + k_4 \mu_1 X_1 \\ \quad + k_5 \mu_2 X_2 + k_7 (k_8 P_{CO_2} + Z - C_{TI} - S_2) \end{cases} \quad (13)$$

where X_1 , X_2 , S_1 , S_2 and C_{TI} are respectively the concentrations of acidogenic bacteria, methanogenic bacteria, COD, Volatile Fatty Acids (VFA) and total inorganic carbon. The variable Z is a measure of the alkalinity (i.e., the chemical buffer capacity). The parameter α represents a proportionality parameter of experimental determination. The variable D_r is the dilution rate and is supposed to be a persisting input, i.e. $\int_0^\infty D_r(\tau) d\tau > 0$. In all cases, the upper index i indicates "influent concentration". In the following, the total inorganic carbon influent concentration C_{TI}^i is omitted due to its weak influence on the anaerobic system.

Like in any other mass balance model of biological processes, a strongly nonlinear kinetic behaviour is present due to the reaction rates. These rates are given by $\mu_1 = \mu_{1max} \frac{S_1}{K_{S1} + S_1}$ where μ_{1max} is the maximum bacterial growth rate and K_{S1} the half

saturation constant associated with the substrate S_1 and $\mu_2 = \mu_{2max} \frac{S_2}{S_2 + K_{S2} + \left(\frac{S_2}{K_{I2}}\right)^2}$ where μ_{2max}

is the maximum bacterial growth rate without inhibition, K_{S2} and K_{I2} are the saturation and inhibition constants associated with the substrate S_2 , respectively. The CO_2 partial pressure P_{CO_2} is expressed as a function of the states as

$$P_{CO_2} = \frac{\phi - \sqrt{\phi^2 - 4k_8 P_T [CO_2]}}{2k_8} \quad \text{where}$$

$$\phi = k_8 P_T + [CO_2] + \frac{k_6 \mu_2 X_2}{k_7} \quad \text{and}$$

$$[CO_2] = C_{TI} + S_2 - Z.$$

The model takes the following classical state space representation as :

$$\dot{\xi} = Kr(\xi) - D\xi + F - Q \quad (14)$$

$$\begin{aligned} \text{where } \xi &= [X_1 \ X_2 \ Z \ S_1 \ S_2 \ C_{TI}]^T, \\ r(\xi) &= \begin{bmatrix} \mu_1(\xi) X_1 \\ \mu_2(\xi) X_2 \end{bmatrix}, \quad K^T = \begin{bmatrix} 0 & 10 & 0 & -k_3 & k_5 \\ 100 - k_1 & k_2 & k_4 \end{bmatrix}, \\ F^T &= [0 \ 0 \ D_r Z^i \ D_r S_1^i \ D_r S_2^i \ 0], \quad Q^T = [0 \ 0 \ 0 \ 0 \ 0 \ Q_{CO_2}] \\ \text{and } D &= \text{diag}(\alpha D_r, \alpha D_r, D_r, D_r, D_r, D_r). \end{aligned}$$

In this study, it can be noticed that many process variables are measured on the process. S_1 , S_2 , Z , Q_{CO_2} and Q_{CH_4} represent the available measurements on the process. The output vector is denoted Y and is related to the state of the system by a nonlinear equation.

Thus, the mathematical model of the reactor for the treatment of industrial wine distillery vinasses takes the following discrete non linear state space representation:

$$\begin{aligned} \xi(k+1) &= F(\xi(k), U(k), \xi_{in}(k)) + W(k) \\ Y(k) &= G(\xi(k)) + V(k) \end{aligned} \quad (15)$$

where $\xi \in \mathfrak{R}^6$ ($\xi = [X_1 \ X_2 \ Z \ S_1 \ S_2 \ C_{TI}]^T$) is the state vector, $u \in \mathfrak{R}^1$ ($u = D_r$) is the control input vector, $\xi_{in} \in \mathfrak{R}^3$ ($\xi_{in} = [D_r S_1^i \ D_r S_2^i \ D_r Z^i]^T$) is the unknown input vector and $Y \in \mathfrak{R}^5$ $Y = [S_1 \ S_2 \ Z \ Q_{CH_4} \ Q_{CO_2}]^T$ is the output vector. $F(\cdot)$ represents the nonlinear state function described by equation (13) and $H(\cdot)$ represents the nonlinear measurement function.

4.3 Results and comments

It is worth noting that the real pilot plant in extreme cases can be destabilised. An overloading of influent concentration can lead to catastrophic consequences in downstream biological process: the system becomes "unstable". Consequently, the simulation, based on the dynamic model of the pilot plant, is used within the framework of the above developed

full-order Kalman filter based on multiple model representation. Note that some previous studies (Bernard *et al.*, 1998) have established that the model reproduces precisely the behaviour of the system and the simulation also correctly reproduces the effect of the perturbation. For illustration purposes, three linear models, established around each operating point, are considered in the following study. Three discrete linear stochastic models, according to (2) obtained for a sampling period of five minutes, are directly defined according to the dilution rate D_r from the nonlinear system representation (15). In order to investigate the performances of the proposed multiple model scheme, the estimation results (both concerning the unmeasured states and inputs) are shown using two different sets of initial conditions summarised in Table 2.

Table 2. Initial conditions

	$X_1(0)$	$X_2(0)$	$C_{TI}(0)$
Real system	1.4	0.22	52
	$\hat{X}_1(0)$	$\hat{X}_2(0)$	$\hat{C}_{TI}(0)$
Set 1	1.25	0.19	46
Set 2	1.54	0.24	57

The results shown in the figures in the last page are responses with respect to set-point changes. In the simulation, a gaussian noise ($N(0,1e-4^2)$) is added to each output signal. Firstly, the validation of the isolation procedure is shown in figure 2 where step variation D_r is considered for a range of 8000 samplings with a sampling period equal to five minutes.

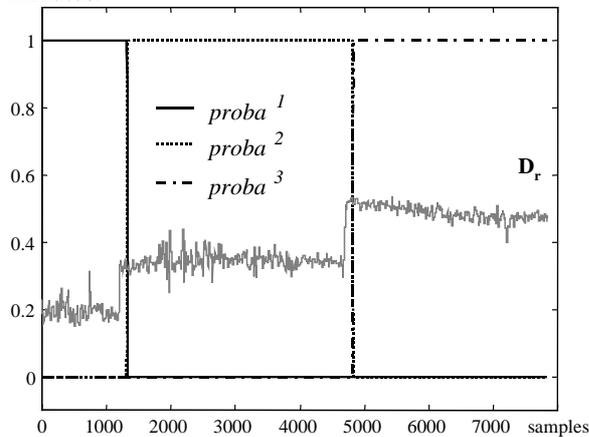


Fig. 2. Time evolution of Mode probabilities and Dilution rate

Based on a bank of 3 unknown inputs Kalman filters, the mode probabilities of each model exactly correspond to the operating values. The selected model is always close to the dynamic behaviour of the non linear system according to the considered operating regimes. Therefore, the following Fig. 3, 4, 5, 6, 7 and 8 show the good convergence properties of the estimator for the different initial values.

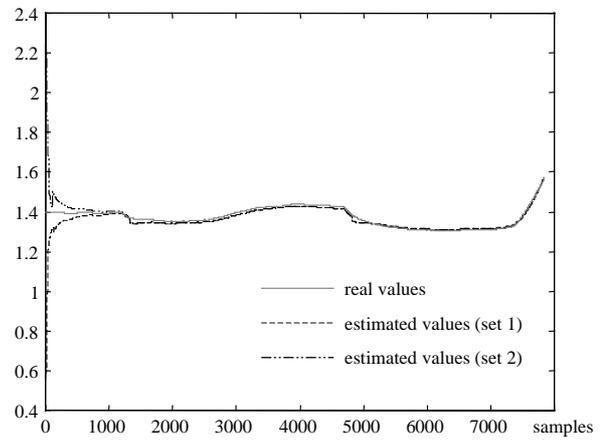


Fig. 3. The unmeasured state X_1 and \hat{X}_1 (g/l)

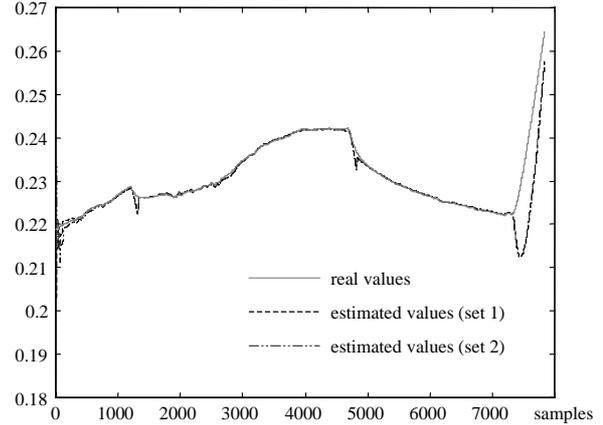


Fig. 4. The unmeasured state X_2 and \hat{X}_2 (g/l)

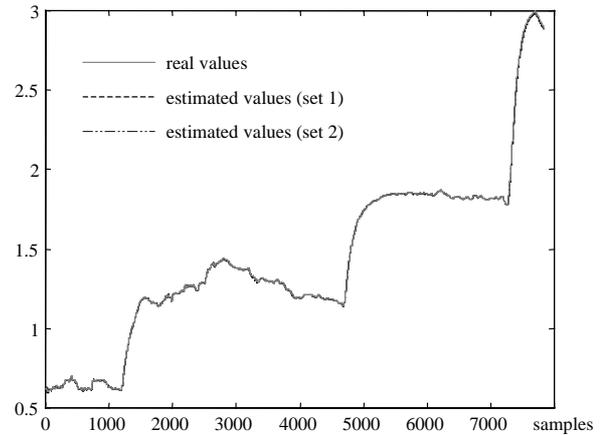


Fig. 5. The unmeasured state C_{TI} and \hat{C}_{TI} (g/l)

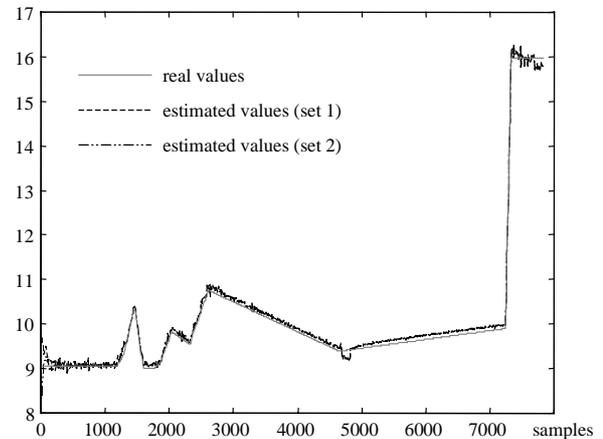


Fig. 6. The unmeasured inputs S_1^i and \hat{S}_1^i

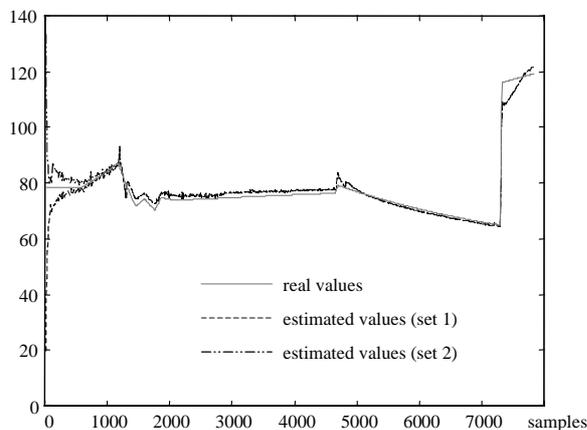


Fig. 7. The unmeasured inputs S_2^i and \hat{S}_2^i

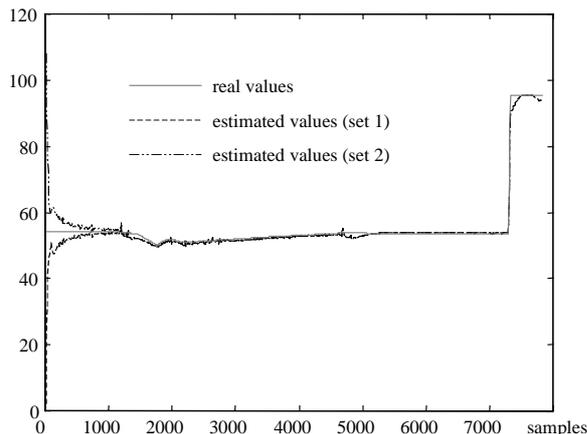


Fig. 8. The unmeasured inputs Z^i and \hat{Z}^i

These different time evolution illustrate the potential of the proposed approach to estimate unmeasured states and inputs. For each operating point, the bank of full-order Kalman filters provides unknown inputs estimation. Those estimations are optimally decoupled from the state. Nevertheless, the proposed method requires an exact knowledge of the number of linear models describing the complete dynamic behaviour of the non linear system.

Finally, notice that the performances of the multiple model scheme are comparable whatever are the uncertainty considered on the initial conditions as presented in the different figures. It is worth noting that the sensitivity of the unknown inputs estimation to the noise measurements was not evaluated in this simulation but it is possible to see the influence of noise measurements on the unknown inputs.

5. CONCLUSION

In this paper an estimation filter has been designed for the monitoring of an anaerobic digestion pilot plant. The estimation of the input concentrations of Wastewater Treatment Plants is a very challenging problem. Recall that these systems suffer of a quasi systematic lack of sensors and that their investment (and operating) costs and the presence of suspended solids in the influent usually limit their practical implementation. The approach uses the concept of a bank of unknown input Kalman filtering according to the assumption that the dynamic of the discrete non linear system could be defined as a combination of discrete linear invariant model. It was shown that

satisfying results were obtained under the assumptions that the system is operating around nominal conditions. The procedure is quite simple to implement nevertheless it requires a dynamical model of the process.

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