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Modelling and Identification of an Activated Sludge Depollution Bioprocess

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Abstract: - In this work the problem of modelling and identification of an activated sludge depollution bioprocess is focused. This bioprocess is in fact an aerobic fermentation process that is carried out in a recycle bioreactor. A nonlinear dynamical model is obtained using the reaction scheme and the mass balance. The dynamical kinetics of the process are strongly nonlinear and not exactly known; therefore an estimation strategy is developed for identification. The nonlinear observer design is based on high gain approach. The tuning of the observers is reduced to the calibration of a single parameter. Computer simulations are included.

Key-Words: - Wastewater treatment, Biotechnology, Nonlinear systems, Identification, High gain observers

1 Introduction

Nowadays the use of advanced control for wastewater treatment plants is low. A main reason is the lack of quality of the data, and the fact that more sophisticated control strategies must be based on a model of the dynamics of the process [1], [4], [8]. When biotechnology strategies are used in wastewater treatment, the nonlinearity of the bioprocesses and the absence of cheap and reliable instrumentation require an enhanced modelling effort and modern identification strategies for the kinetics. In order to apply modern control strategies, it is necessary to obtain useful models. Many times, the dynamic models are high-order and nonlinear. Reduced-order techniques must to be applied for these models. Serious problems appear in the measurement of substrates, biomass, and product concentrations. In many cases the state variables, i.e. the concentrations, were analysed manually and as a result there is not on-line (and real-time) control.

These problems can be solved using "software sensors". A software sensor is a combination between a hardware sensor and a software estimator. These software sensors are used not only for the estimation of the concentrations - the state variables - but also for the estimation of the kinetic parameters. Very important is the estimation of kinetic rates inside a bioreactor - the estimates of these rates are used for advanced control strategies. The interest for development of software sensors for bioreactors is proved by the big number of publications and applications in this area [1], [5], [8], [10], [12]. The first approach from historically point of view is based on Kalman filter which leads to complex nonlinear algorithms. Another well-known technique is the Bastin and Dochain approach based on the adaptive systems theory [1]. This strategy consists in the estimation of unmeasured state with asymptotic observers, and after that, the measurements and the estimates of the state variables are used for on-line estimation of kinetic rates. Remarkable is the fact that the state asymptotic observers are designed without any knowledge of kinetics. This method is useful, but in some cases, when many reactions are involved, the implementation requires the calibration of too many parameters. For example, if we have n components' concentrations used for the estimation of m kinetic rates, is necessary to calibrate $2n$ tuning parameters. For overcome this problem, a possibility is to design an estimator using a high gain approach (see [2], [5], [6], [10]). The gain expression of these observers involves a single tuning parameter whatever the number of components and reactions.

This paper is organized as follows. An important wastewater treatment process - the activated sludge process - is presented in Section 2. The bioprocess is carried out in a Continuous Stirred Tank Bioreactor (CSTB) with recycle stream. The reduced model of the process is obtained using the singular perturbations approach. Section 3 deals with the design of an on-line estimation strategy for the identification of the unknown kinetics. The on-line estimation algorithm is based on high gain technique. Computer simulations illustrate the performances of nonlinear observers. Finally, concluding remarks are collected in Section 4.

2 Dynamical model of the activated sludge bioprocess

A bioreactor is a tank in which several biological reactions occur simultaneously in a liquid medium [1]. A biotechnological process carried out in a bioreactor can be defined as a set of *m* biochemical reaction involving *n* components. In industry, the bioreactors operate in three modes: the continuous mode, the fed-batch mode and the batch mode [1], [10]. Bioreactors that operate in the continuous mode are usually known as Continuous Stirred Tank Bioreactors. In a CSTB, the substrates (the nutrients) are fed to the bioreactor continuously and an effluent stream is continuously withdrawn from the CSTB such that the culture volume is constant. Often, a part of the biomass is recycled. To recycle, the biomass must be separated from the substrate and yield, then travel through pipes after separation. This time of recycle introduce delays in the states and complicates the dynamics. The benefits are that the recycle increases the overall conversion and reduces the costs.

The activated sludge process is an aerobic process of biological wastewater treatment [1], [4]. It is usually operated in at least two interconnected tanks, Fig. 1: an aerator in which the biological degradation of the pollutants takes place and a sedimentation tank (settler) in which the liquid is clarified, that is the biomass is separated from the treated wastewater. Part of the settled biomass is fed back to the bioreactor, while the surplus biomass is removed from the process. The reaction in the aerator may be described by a simple autocatalytic aerobic microbial growth that can be represented by the following scheme:

$$k_1 S + k_2 C \xrightarrow{\varphi \leftarrow} X \tag{1}$$

where *S*, *X* and *C* are respectively the pollutants, the biomass and the dissolved oxygen, φ is the reaction rate and k_1 and k_2 are the yield coefficients. The above reaction scheme is a simply qualitative relation and does not include stoichiometric considerations.

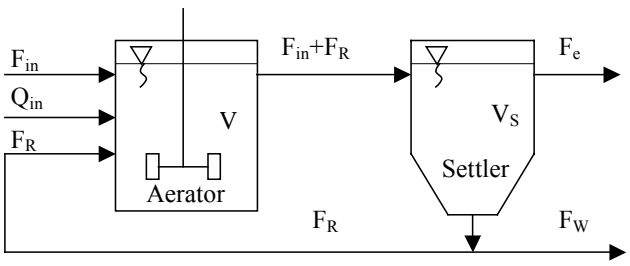

Fig.1. Schematic view of an activated sludge process

It is often assumed that the settler work perfectly, i.e. there is no biomass in the overflow of the settler. Then, the dynamics of the plant (aerator + settler) is described by the following mass balance equations [1], [3], [9]:

$$\begin{aligned}
\frac{dS}{dt} &= -k_1 \mu X - \frac{F_{in} + F_R}{V} S + \frac{F_{in}}{V} S_{in} \\
\frac{dC}{dt} &= -k_2 \mu X - \frac{F_{in} + F_R}{V} C + Q_{in} \\
\frac{dX}{dt} &= \mu X - \frac{F_{in} + F_R}{V} X + \frac{F_R}{V} X_R \\
\frac{dX_R}{dt} &= \frac{F_{in} + F_R}{V_S} X - \frac{F_R + F_W}{V_S} X
\end{aligned} \tag{2}$$

where S_{in} is the concentration of influent substrate (g/l), Q_{in} is the oxygen feed rate (g/lh), X_R is the concentration of the recycled biomass (g/l), F_{in}, F_R and F_W are the influent, recycle and waste flow rates (l/h), respectively, V and V_S the aerator and settler volumes (l), respectively, and $\mu(\cdot)$ is the specific growth rate (h^{-1}) of reaction φ. If we define by $\xi = [S\ C\ X\ X_R]^T$ the state vector of (2), $\varphi = \mu(\cdot)X$ the reaction rate, $F = [D_{in} S_{in}\ Q_{in}\ 0\ 0]^T$ the feed rate vector, $Q = [0\ 0\ 0\ 0]^T$ the gaseous outflow rate vector and $K = [-k_1\ -k_2\ 1\ 0]^T$ the yield coefficient matrix, then the dynamical model (2) can be compactly written as:

$$\dot{\xi} = K\varphi(\xi) - D\xi + F - Q \tag{3}$$

This model describes in fact the dynamics of a large class of bioprocesses carried out in stirred tank bioreactors and is referred as *general dynamical state-space model* of this class of bioprocesses [1]. In (3), D stand for the dilution rate matrix and is given by

$$D = \begin{bmatrix} D_1 & 0 & 0 & 0 \\ 0 & D_1 & 0 & 0 \\ 0 & 0 & D_1 & -D_R \\ 0 & 0 & -D_2 & -D_3 \end{bmatrix} \tag{4}$$

whose entries are defined as:

$$\begin{aligned}
&D_{in} = \frac{F_{in}}{V}, \quad D_R = \frac{F_R}{V}, \quad D_1 = D_{in} + D_R, \\
&D_2 = \frac{F_{in} + F_R}{V_S}, \quad D_3 = \frac{F_R + F_W}{V_S}
\end{aligned} \tag{5}$$

The oxygen feed rate Q_{in} is usually set equal to the liquid-gas oxygen transfer rate:

$$Q_{in} = k_L a \cdot (C_s - C) \tag{6}$$

where $k_L a$ is the oxygen mass transfer coefficient and C_s the saturation constant. In the following, we shall consider that $k_L a$ is a linear function of the air flow rate W [3]:

$$k_L a = a_0 W, \quad a_0 > 0 \tag{7}$$

The most difficult task for the construction of the dynamical model (3) is the modelling of the reaction kinetic φ. The form of kinetics is complex, nonlinear and in many cases partial or completely unknown. A realistic assumption is that a reaction can take place only if all reactants are presented in the bioreactor. Therefore, the reaction rates are necessarily zero whenever the concentration of one of reactants is zero. A common form for the reaction rate is $\varphi = \mu(\cdot)X$. A possible structure of the nonlinear specific growth rate $\mu(\cdot)$ is a Monod-type model, i.e. [9]:

$$\mu(S,C) = \mu_{\max} \frac{S}{K_S + S} \cdot \frac{C}{K_C + C} \tag{8}$$

where $\mu_{\max}$ is the maximum specific growth rate and K_S, K_C are Michaelis-Menten coefficients.

The model order can be reduced using singular perturbations techniques [7]. A systematic approach to model order reduction via singular perturbation for bioprocesses is fully described in [1]. Let's consider that there are low-solubility products and/or substrates that occur only in fast reactions. In the general dynamical model (3) each of them is denoted ξ_i and its corresponding dynamical equation is:

$$\frac{d\xi_i}{dt} = -D\xi_i + K_i\varphi + F_i - Q_i \tag{9}$$

where K_i is the line of K corresponding to ξ_i. Then, application of singular perturbation result in setting ξ_i and $d\xi_i / dt$ to zero and replacing the dynamical equation (9) by the algebraic equation:

$$K_i\varphi = Q_i - F_i \tag{10}$$

Another typical situation of application of singular perturbations to biosystems control is the multi-reactor case when the volumes of tanks are quite different from one another. For instance, in the activated sludge process, the dynamics of X_R can be written as follows:

$$\frac{V_S}{V}\frac{dX_R}{dt} = (D_{in} + D_R)X - (D_R + D_{VW})X_R \tag{11}$$

with $D_{VW} = F_W / V$. If V_S is small with respect to V, V_S / V may be considered as being negligible. Singular perturbations consist of setting V_S / V to zero and replacing (11) by the following algebraic equation:

$$(D_{in} + D_R)X = (D_R + D_{VW})X_R \tag{12}$$

So, the order of the model is reduced from 4 to 3 and the reduced-order model can be used in estimation or control strategies. This reduced-order model consists of the first three equations of the model (2), where the concentration of the recycled biomass X_R is replaced using the algebraic equation (12). Then the state vector of the reduced-order model becomes $\xi_r = [S\ C\ X]^T$.

3 High gain observers and simulation results

3.1 Design of the high gain observers

When the parameters and the kinetics of the bioprocess are partially known or unknown, it is necessary to use identification procedures. In practice, in the case of the activated sludge bioprocess, the reaction rate φ and the specific growth rate μ are unknown (the form (8) of the specific growth rate is a simple assumption). For on-line estimation of these kinetic rates, algorithms based on a state observer technique or linear regressive observers can de designed [1]. These algorithms provide good estimates for the unknown kinetics, but the problem is the number of tuning parameters ($2 \times n$). In order to overcome this disadvantage, a simple nonlinear observer based on high gain approach is proposed in [2], [5], [6].

In order to design high gain observers for the unknown kinetics, the reduced-order model of the activated sludge bioprocess will be written as:

$$\frac{d\xi_r}{dt} = K_r \cdot H(\xi_r) \cdot \rho(t) - D_r \cdot \xi_r + F_r \tag{13}$$

with

$$K_r = \begin{bmatrix} -k_1 \\ -k_2 \\ 1 \end{bmatrix};\ D_r = \begin{bmatrix} D_1 & 0 & 0 \\ 0 & D_1 & 0 \\ 0 & 0 & D_1 - D_0 \end{bmatrix};$$
$$F_r = \begin{bmatrix} D_{in} S_{in} \\ a_0 (C_S - C) W \\ 0 \end{bmatrix};\ D_0 = D_R \frac{D_R + D_{in}}{D_R + D_{VW}}$$

In (13), $\rho(t)$ represents the unknown kinetics of the process. If we suppose that the reaction rate is totally unknown, then $\rho(t) = \varphi(t)$ and $H(\xi_r) = 1$. If the structure of the reaction rate is known: $\varphi = \mu(\cdot)X$, but the specific growth rate is unknown, then $\rho(t) = \mu(t)$ and $H(\xi_r) = X$.

For the model (13), the yield matrix (vector in our particular case) K_r, with $\dim(K_r) = 3 \times 1$, is of full rank, i.e. $rank(K_r) = 1$. This assumption is true for our particular model, and for the general class (3) case is a generic property of the yield matrix. We shall suppose that all state variables are measured (contrarily, a state estimator can be used). Since K_r is full rank, i.e. is left invertible, a full rank arbitrary submatrix K_a (in our particular case a scalar) of K_r can be considered. Let K_b be the remaining submatrix of K_r. Then the system (13) can be written as follows:

$$\begin{aligned} \dot{\xi}_a &= K_a \cdot H(\xi_a, \xi_b) \cdot \rho(t) - D_a \cdot \xi_a + F_a \\ \dot{\xi}_b &= K_b \cdot H(\xi_a, \xi_b) \cdot \rho(t) - D_b \cdot \xi_b + F_b \end{aligned} \tag{14}$$

where (ξ_a, ξ_b), (F_a, F_b) and (D_a, D_b) are partitions induced by the factorization of K_r.

We suppose $\xi_b(t)$ a known (measured) signal, denoted $\sigma(t) = \xi_b(t)$. Then consider the system [5]:

$$\begin{aligned} \dot{\xi}_a &= K_a \cdot H(\xi_a, \sigma) \cdot \rho(t) - D_a \cdot \xi_a + F_a \\ \dot{\rho} &= g(t) \end{aligned} \tag{15}$$

where *g(t)* is a bounded unknown function, which may depend on ξ_a, σ, inputs, noise. The hypothesis of boundedness of the kinetics is in accordance with industrial practice. The design of nonlinear high gain observers is done in [2], [5], [6]. The high gain observer equations for the general class of bioprocesses (3) and applicable also for the activated sludge process described by (13) are [5], [11]:

$$\begin{aligned} \dot{\hat{\xi}}_a &= K_a H(\hat{\xi}_a, \sigma)\hat{\rho} - D_a \hat{\xi}_a + F_a - 2\theta(\hat{\xi}_a - \xi_a) \\ \dot{\hat{\rho}} &= -\theta^2 \cdot \left[K_a \cdot H(\hat{\xi}_a, \sigma)\right]^{-1} \cdot (\hat{\xi}_a - \xi_a) \end{aligned} \tag{16}$$

The observer (16) provides on line estimates $\hat{\rho}$ for the unknown kinetics; this observer is in fact a copy of the bioprocess model, but with the state ξ_a replaced by its estimate $\hat{\xi}_a$, and with a corrective term. The tuning of this observer is very simple because a single parameter is involved: θ.

For the activated sludge bioprocess, the factorization of yield matrix K_r is:

$$K_a = -k_1 \tag{17}$$

and consequently we obtain:

$$\begin{aligned} &\xi_a = S;\ \xi_b = \sigma = \begin{bmatrix} C \\ X \end{bmatrix};\ K_b = \begin{bmatrix} -k_2 \\ 1 \end{bmatrix}; \\ &F_a = D_{in} S_{in};\ F_b = \begin{bmatrix} a_o (C_S - C) W \\ 0 \end{bmatrix}; \\ &D_a = D_1;\ D_b = \begin{bmatrix} D_1 & 0 \\ 0 & D_1 - D_0 \end{bmatrix} \end{aligned} \tag{18}$$

From equations (13), (16), and with the factorization (17), (18), we can obtain the equations of two high gain observers:

(i) an observer for on-line estimation of the reaction rate $\rho(t) = \varphi(t)$ (with $H(\xi_r) = 1$):

$$\begin{aligned} \frac{d\hat{S}}{dt} &= -k_1 \cdot \hat{\varphi} - D_1 \cdot \hat{S} + D_{in} S_{in} - 2 \cdot \theta \cdot (\hat{S} - S) \\ \frac{d\hat{\varphi}}{dt} &= -\theta^2 \cdot \left[-k_1\right]^{-1} \cdot (\hat{S} - S) \end{aligned} \tag{19}$$

(ii) an observer for on-line estimation of the specific growth rate $\rho(t) = \mu(t)$ (with $H(\xi_r) = X$):

$$\begin{aligned} \frac{d\hat{S}}{dt} &= -k_1 \cdot X \cdot \hat{\mu} - D_1 \hat{S} + D_{in} S_{in} - 2 \cdot \theta \cdot (\hat{S} - S) \\ \frac{d\hat{\mu}}{dt} &= -\theta^2 \cdot \left[-k_1 \cdot X\right]^{-1} \cdot (\hat{S} - S) \end{aligned} \tag{20}$$

Remark. It can be seen that the estimator (19) needs only the measurements of *S*, and the estimator (20) needs both measurements of *S* and *X*.

3.2 Simulation results

The performances of the nonlinear observers have been tested by performing extensive simulation experiments. The activated sludge process has been simulated by numerical integration of the basic dynamical model equations (13), considering the

specific growth rate μ as a Monod-type model (8) with: $\mu_{\max} = 0.2\,h^{-1}$, $K_S = 75\,mg/l$, $K_C = 2mg/l$, and the following bioprocess parameters [3], [11]:

$$k_1 = 1.2, k_2 = 0.565, a_0 = 0.018m^{-3}, C_S = 10\,mg/l,$$
$$V = 100m^3, V_S = 50\,m^3, F_{in} = 15m^3/h,$$
$$F_W = 0.5m^3/h, F_R = 10m^3/h, W = 100m^3/h.$$

The equations (13) were integrated under the following initial conditions: $S = 5mg/l, C = 6mg/l$, $X = 1.25g/l, X_R = 2.5\,g/l$.

The nonlinear high gain observers (19), (20) were implemented for the activated sludge process (13). The simulations are performed considering that the reaction rate φ for the first observer and the specific growth rate μ for the second observer are unknown. We consider that the influent substrate concentration S_{in} is a disturbance applied to the bioreactor, with the time profile plotted in Fig. 2.

In the case of first estimator (19), the main goal is to reconstitute the time evolution of φ from the measurements of *S*, and for the second observer (20) the objective is to reconstitute the time evolution of μ using the measurements of *S*, *X* (in fact obtained from simulation). The "true" values of the specific growth rate (8) are used only for the simulation of measured data from the bioprocess. Fig. 3 shows the evolutions of state variables, respectively, *S* (mg/l) and *C* (mg/l); in Fig. 4 the time profile of the biomass concentration *X* (g/l) is depicted. In Fig. 5 the estimated parameter $\hat{\rho} = \hat{\varphi}$ and the real reaction rate φ are presented (the observer (i)). Fig. 6 depicts the time evolution of the estimated rate $\hat{\rho} = \hat{\mu}$ and the real specific growth rate μ (the observer (ii)). The tuning parameter was set to the value $\theta = 10$.

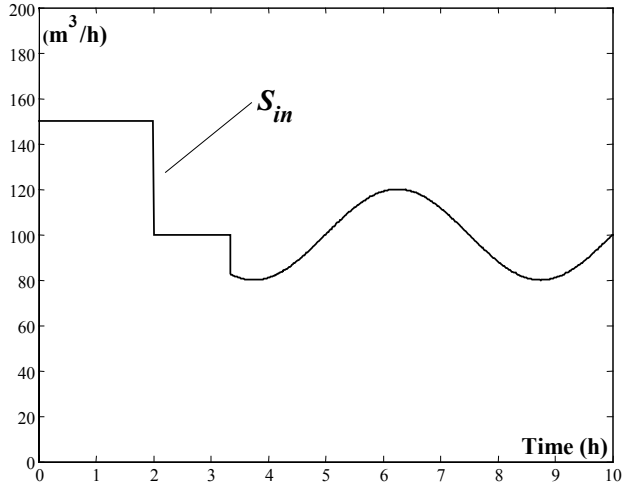

Fig. 2. Time profile of the disturbance S_{in}

Finally, in order to test the robustness of the nonlinear observers to noisy measurements, the measurement of *X* is vitiated by an additive Gaussian noise (see Fig. 4). This noise is with zero mean and amplitude equal to 5% of the free noise values. In Fig. 7 the specific growth rate and its estimate obtained using noisy data of *X* are depicted. In all figures, the values obtained from simulation are depicted with solid curves and the estimates with dashed curves. Notice that the estimation error can be made as small as wished if we choose greater values of θ. The problem for a large value of θ is that the observer becomes noise sensitive.

The results obtained for both estimators can be substantially improved if the tuning parameter is chosen higher in value. This relative big value of θ can be used only if the measurements are free-noise. Contrarily is possible that the estimates of kinetics cannot be utilised. The value of the tuning parameter is therefore a compromise between a good estimation and the noise rejection.

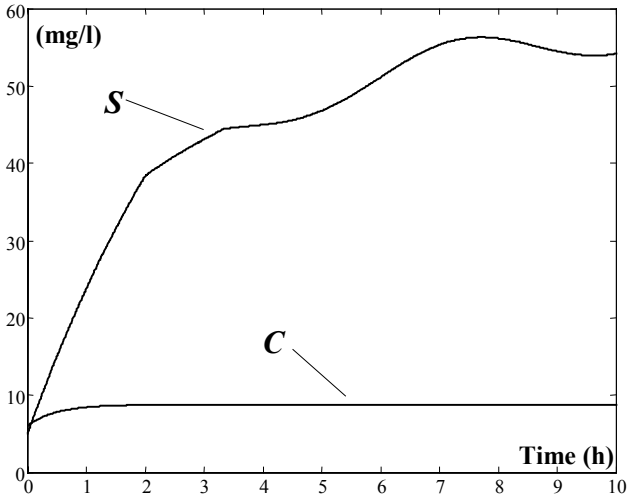

Fig. 3. Time evolution of substrate and dissolved oxygen concentrations

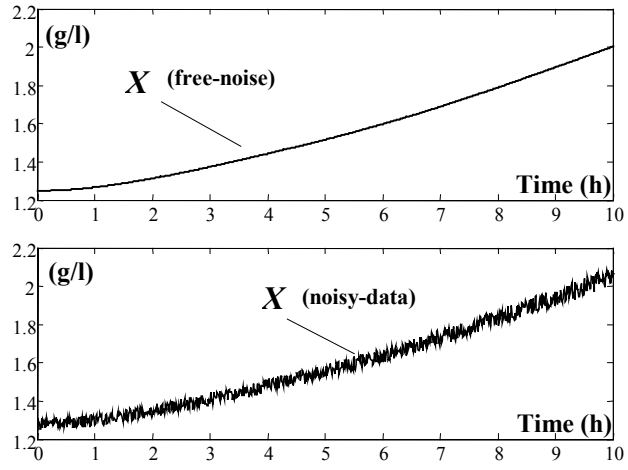

Fig. 4. The evolution of the biomass concentration

4 Conclusions

Some aspects regarding the modelling and the identification of an activated sludge depollution bioprocess have been presented in this work. The dynamic nonlinear model of this bioprocess that takes place in a recycle bioreactor was widely analysed and the singular perturbations theory was applied to facilitate the order reduction of the model.

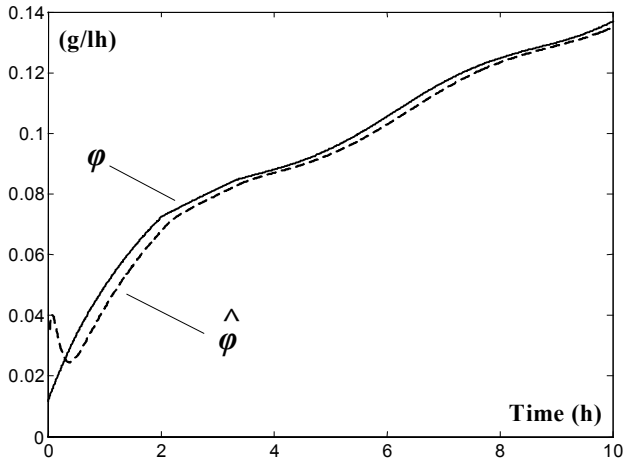

Fig. 5. Time profiles of reaction rate and its estimate

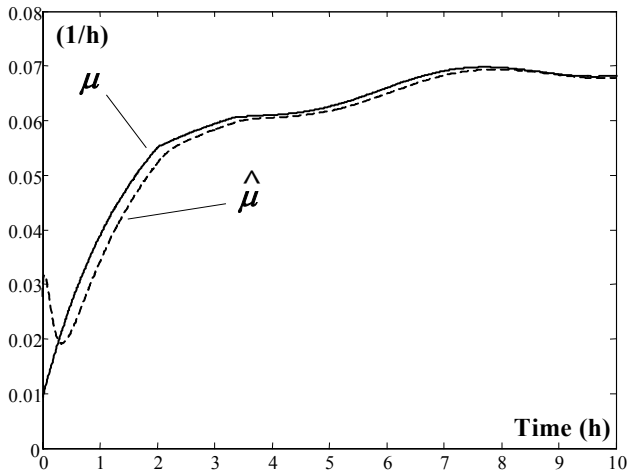

Fig. 6. The real and estimated specific growth rate

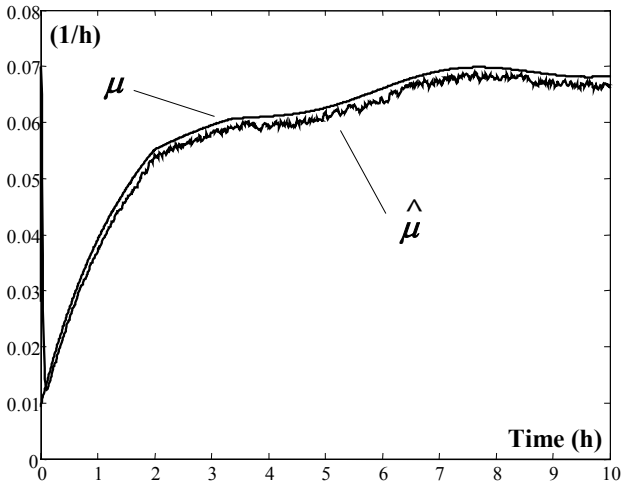

Fig. 7. Time evolution of μ, $\hat{\mu}$ – noisy data of X

The design and the implementation of simple nonlinear high gain observers for the activated sludge process was examined. The high gain observers allow on-line estimation of the unknown kinetic rates inside the bioreactor. The calibration of these observers is simple because implies the tuning of a single parameter whatever the number of components and reactions. The observers proposed for the depollution bioprocess need measurements of a part of the state variables. Anyhow, if it is no possible to measure on-line these concentrations, a state estimator is needed. Good results are obtained via simulation. The estimation results can be utilised for the control purposes.

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