

Nonlinear on-line Estimation and Adaptive Control of a Wastewater Treatment Bioprocess

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Introduction

Today, the exploitation of modern control strategies for bioprocesses, and in particular for wastewater treatment processes, is hindered by some problems [1–3]: the nonlinearity of dynamics, uncertainty of process parameters, and absence of cheap and reliable instrumentation. The aerobic treatment of wastewater by activated sludge is a common process, but the characteristics of a lot of industrial emissions frequently cause operational problems in continuous flow systems [4, 5]. As a result, discontinuous processes such as biological Sequencing Batch Reactors (SBRs) can be taken into consideration due to the fact that they could operate better than the continuous processes, in terms of operation costs, process stability, and reliability [4, 5].

A key issue for bioprocesses is the estimation of state variables and of parameters, especially of the kinetic rates [4]. This problem can be solved using the so-called “software sensors”, which are combinations between hardware sensors and software estimators [1, 2, 6]. Presently, two classes of state observers for bioprocesses are applied frequently [1–7]: classical nonlinear observers, based on a perfect knowledge of the model structure, and asymptotic observers, for which the design is based on mass and energy balances without the knowledge of process kinetics being necessary.

Concerning the kinetic parameters estimation, a well-known technique is the approach based on adaptive systems theory [6]. This technique consists in the estimation of unmeasured states with asymptotic observers, and after that, the measurements and the state estimates are used for on-line estimation of kinetics. This useful method was applied for SBRs [4], but in some cases, when many reactions are involved, it requires the calibration of many parameters. In order to surmount this problem, a possibility is to design an estimator using a high-gain approach [8–11], which involves a single tuning parameter, whatever the number of reactions and components.

Several bioprocess control strategies were developed, such as sliding mode control [7], adaptive control [2, 6], optimal control, vibrational control, fuzzy and neural strategies, and so on. For wastewater treatment bioprocesses taking place into fed-batch reactors, the adaptive control approach is a viable alternative of the optimal control [2, 6].

This paper, which is an extended work of [10, 12], addresses on-line estimation and control issues for a typical wastewater treatment bioprocess. The polluted water comes from the chemical industry, containing toxic or recalcitrant compounds; this biotechnological process was studied in detail by Fibrianto *et al.* [4], Buitron *et al.* [5], in the frame of an EC project – EOLI. In the present work, a model derived in the frame of this project will be used. More precisely, the model EM1 will be used, which represents a process taking place inside a fed-batch bioreactor, with one aerobic growth reaction and an endogenous respiration reaction [4].

In order to design a control law, the so-called exact linearizing approach is used. The nonlinear controller thus obtained is combined with an estimator for the unknown kinetics, i.e. the reaction rates of the bioprocess. This estimator is based on high-gain approach (Gauthier *et al.* [9], Farza *et al.* [8]). Due to the fact that the implementation of high-gain observer and of the adaptive controller requires on-line state estimates, these will be provided by an asymptotic observer. The performance and the behavior of estimation and control algorithms are studied by using extensive numerical simulations.

The advantages of the proposed adaptive control scheme with respect to other similar approaches are the simplicity (only two tuning parameters are used for the estimation and control algorithms), and the robustness against perturbations (noisy measurements, parametric disturbances).

The organization of the paper is as follows. In Section 2, the dynamical model of the wastewater treatment process is presented. The next section deals with the design

of state and parameter estimation algorithms. The adaptive control approach is studied in Section 4, and in the next section the simulation results are presented. In the last section, concluding remarks are collected.

Nonlinear model of the wastewater treatment process

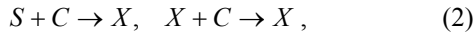
Usually, a bioprocess carried out inside a bioreactor can be defined as a set of m biochemical reactions involving n components (with $n > m$). By using the mass balance of the components and obeying some modeling rules, a dynamical state-space model can be obtained [2, 6]. The model is described by the equations [6]

$$\dot{\xi} = K \cdot \varphi(\xi) - D\xi + F - Q. \quad (1)$$

The vector of instantaneous concentrations is the state vector: $\xi = [\xi_1 \ \xi_2 \ \dots \ \xi_n]^T$. The vector of the reaction rates (the so-called reaction kinetics) will be denoted $\varphi = [\varphi_1 \ \varphi_2 \ \dots \ \varphi_m]^T$. $K = [K_{ij}]$, $i = \overline{1, n}, j = \overline{1, m}$ is the so-called matrix of the yield coefficients and D is the specific volumetric outflow rate, usually called dilution rate. $F = [F_1 \ F_2 \ \dots \ F_n]^T$ is the vector of supply rates, and $Q = [Q_1 \ Q_2 \ \dots \ Q_n]^T$ is the vector of removal rates of the components in gaseous form. The nonlinear model (1) describes in fact the behavior of an entire class of bioprocesses and is referred to as the general dynamical state-space model of this class [2, 6]. In (1), the term $K \cdot \varphi(\xi)$ represents the reaction kinetics, and the term $-D\xi + F - Q$ is the exchange with the environment.

The strongly nonlinear character of this model is given by the reaction kinetics. In practice, the yield coefficients, the structure and parameters of reaction rates are partially known or even completely unknown.

The process considered in the following is the treatment of wastewater from chemical industry, containing toxic or recalcitrant compounds (4-chlorophenol 4CP), which takes place inside a SBR, located at UNAM (Universidad Nacional Autonoma de Mexico), Mexico City [4, 5]. The process consists of an aerobic growth reaction and an endogenous respiration reaction, with the reaction scheme [4]



where S , C and X are the organic matter (substrate), dissolved oxygen and biomass, respectively. A detailed model of this fed-batch process, referred to as EM1, was obtained after a lot of experiments in [4, 5].

From the reaction scheme (2), using the mass balance equations, and assuming that the dissolved oxygen is not limiting and the biomass decay is negligible, a model expressing the evolution of concentrations is obtained [4]:

$$\begin{cases} \dot{X} = \mu(S)X - DX, \\ \dot{S} = -k_1\mu(S)X + D(S_{in} - S), \\ \dot{C} = -k_2\mu(S)X - bX + D(C_{in} - C) + K_L a(C_S - C), \\ \dot{V} = DV = F_{in}, \end{cases} \quad (3)$$

where $\mu, F_{in}, V, k_1, k_2, S_{in}, C_{in}, b, K_L a$ and C_S are: specific growth rate, inlet flow rate, volume, yield coefficients, influent substrate and dissolved oxygen concentrations, endogenous respiration kinetic coefficient, gas-liquid transfer coefficient, and oxygen saturation concentration.

The ratio $D = (F_{in} / V)$ is the dilution rate, and $\varphi = \mu(S)X$ is the reaction rate. If the first three equations of (3) are considered, using the notations $\xi = [X \ S \ C]^T$ - state vector, $F = [0 \ DS_{in} \ DC_{in}]^T$ - the vector of supply rates, $K = [1 \ -k_1 \ -k_2]^T$ - the yield vector, and $\tilde{Q} = [0 \ 0 \ bX - K_L a(C_S - C)]^T$ - the extended vector of removal rates, then a model of the form (1) is obtained

$$\dot{\xi} = K \cdot \varphi(\xi) - D\xi + F - \tilde{Q}. \quad (4)$$

The specific growth rate can be modeled as Haldane law that considers the substrate inhibition on growth [1, 2]

$$\mu(S) = \mu^* S / (K_S + S + S^2 / K_I), \quad (5)$$

with μ^* - maximum specific rate, K_S - Michaelis-Menten constant; K_I an inhibition constant.

Considering the particular case of the biotechnological process (4), often the only on-line available state variable is the dissolved oxygen concentration [4]. Furthermore, the nonlinear expression of the parameter (5) is uncertain; in fact, this reaction kinetics is imprecisely known. Therefore, for control purposes, an estimation algorithm is required in order to estimate the specific growth rate, using the on-line measurements of dissolved oxygen concentration.

The design of nonlinear estimation algorithms

In order to implement control strategies, when the parameters and kinetics of bioprocess are partially known or unknown, it is necessary to use on-line estimation techniques. In practice, the reaction rates φ and the specific growth rates μ are unknown. For on-line estimation of these kinetic rates, algorithms based on a state observer technique or linear regressive observers can be designed [1, 2, 6]. These algorithms provide good estimates for the unknown kinetics, but the problem is the number of tuning parameters. To overcome this drawback, a simple nonlinear observer based on high-gain approach is proposed in [8, 9].

To facilitate the design of high-gain observers for the unknown kinetics, the general dynamical state-space model (4) of the bioprocesses can be rewritten as

$$\dot{\xi} = K \cdot H(\xi) \cdot \rho(t) - D \cdot \xi + F - \tilde{Q}(\xi), \quad (6)$$

where $\rho(t)$ represents the unknown kinetics of the process. If we suppose that the reaction rate is totally unknown, then $\rho(t) = \varphi(t)$ and $H(\xi) = 1$.

For the model (6), we will suppose that the yield matrix is of full rank. This assumption is true for our model (3), and for the general class (1) is a generic

property of yield matrix. We shall suppose that all state variables are measured (contrarily, a state estimator can be used). Since K is full rank, i.e. is left invertible, a full rank arbitrary submatrix K_a can be considered. Let K_b be the remaining submatrix. Then (6) can be written as:

$$\begin{cases} \dot{\xi}_a = K_a H(\xi_a, \xi_b) \rho(t) - D\xi_a + F_a - \tilde{Q}_a(\xi_a, \xi_b), \\ \dot{\xi}_b = K_b H(\xi_a, \xi_b) \rho(t) - D\xi_b + F_b - \tilde{Q}_b(\xi_a, \xi_b), \end{cases} \quad (7)$$

where (ξ_a, ξ_b) , (F_a, F_b) , $(\tilde{Q}_a, \tilde{Q}_b)$ are partitions induced by the factorization. We suppose $\xi_b(t)$ a known signal, denoted $\sigma(t) = \xi_b(t)$. Then consider the system [8]:

$$\begin{cases} \dot{\xi}_a = K_a H(\xi_a, \sigma) \rho(t) - D\xi_a + F_a - \tilde{Q}_a(\xi_a, \sigma), \\ \dot{\rho} = g(t), \\ w = \xi_a, \end{cases} \quad (8)$$

with $g(t)$ a bounded unknown function, which may depend on ξ_a , σ , inputs, noise.

The design of nonlinear high-gain observers is done in [8, 9], with supplementary assumptions regarding global Lipschitz conditions, the boundedness of $H(\xi)$ diagonal elements' away from zero, etc. The design derives from (8), and consists in calculation of the gain by using an algebraic Lyapunov equation [8]. Then, the equations of the high-gain observer are obtained as follows:

$$\begin{cases} \dot{\hat{\xi}}_a = K_a H(\hat{\xi}_a, \sigma) \hat{\rho} - D\hat{\xi}_a + F_a - \tilde{Q}_a - 2\theta(\hat{\xi}_a - \xi_a), \\ \dot{\hat{\rho}} = -\theta^2 \cdot [K_a \cdot H(\hat{\xi}_a, \sigma)]^{-1} \cdot (\hat{\xi}_a - \xi_a). \end{cases} \quad (9)$$

The high-gain observer (9) provides on-line estimates $\hat{\rho}$ for the unknown kinetics; this observer is in fact a copy of the bioprocess model, with a corrective term. It can be observed that the observer is quite simple and moreover the tuning of the gain can be done by modifying only one design parameter: θ .

Remark 1. Note that in (9), $\hat{\xi}_a$ is an "estimate" of ξ_a , provided by the algorithm in order to be compared with the real state (ξ_a is measured or provided by a state observer), and the resulting error to be used in (9).

Remark 2. When $g(t) = 0$, the nonlinear observer (9) has an exponential convergence of the estimation error. Contrariwise, the estimation error can become arbitrarily small choosing a sufficiently big value for the gain θ .

The general above presented design method can be used for the wastewater treatment bioprocess. We will suppose that the specific growth rate μ is unknown, and the on-line available states are the substrate and dissolved oxygen concentrations. In this particular case we have $\rho(t) = \mu(t)$ the unknown kinetics, and $H(\xi) = X$. The next factorization of yield vector is considered [10, 12]

$$K_a = -k_2, \quad K_b = [1 \ -k_1]^T. \quad (10)$$

Consequently, the following partitions are obtained:

$$\begin{cases} \xi_a = C, \quad \xi_b = \sigma = [X \ S]^T, \quad F_a = DC_{in}, \quad F_b = [0 \ DS_{in}]^T, \\ Q_a = bX - K_L a(C_S - C), \quad \tilde{Q}_b = [0 \ 0]^T. \end{cases} \quad (11)$$

Then, the equations of high-gain observer (9), applied for the wastewater treatment bioprocess are:

$$\begin{cases} \dot{\hat{C}} = -k_2 X \hat{\rho} - D\hat{C} + DC_{in} - bX + K_L a(C_S - \hat{C}) - 2\theta(\hat{C} - C), \\ \dot{\hat{\rho}} = -\theta^2 [-k_2 X]^{-1} (\hat{C} - C). \end{cases} \quad (12)$$

To implement the observer (12), we need the measurements of C , but also of X , which is not on-line available. Hence, an asymptotic observer will be used. The design is based on a change of coordinates, which lead to a submodel of (4) independent of the kinetics [6, 7]. Because we need the estimates of X , we define an auxiliary variable [4]: $z = C + k_2 X$, and from (3) we obtain

$$\dot{z} = -Dz + DC_{in} + K_L a(C_S - C) - (b/k_2)z + (b/k_2)C. \quad (13)$$

Now, the auxiliary variable dynamics is independent of kinetics. The asymptotic observer consists of (13) and the equation obtained by inverting the definition of z

$$X_{est} = (z - C) / k_2. \quad (14)$$

The asymptotic observer (13), (14) is independent of the kinetics and has good convergence and stability performance [2, 6]. The final high-gain equations consist in the relations (12), but with X replaced with the estimate X_{est} provided by the observer (13), (14).

However, if the endogenous respiration kinetic coefficient b is negligible, then a high-gain observer for the reaction rate φ can be designed. In this case, $\rho(t) = \varphi(t)$ and $H(\xi) = 1$. The high-gain observer is defined as:

$$\begin{cases} \dot{\hat{C}} = -k_2 \hat{\rho} - D\hat{C} + DC_{in} + K_L a(C_S - \hat{C}) - 2\theta(\hat{C} - C), \\ \dot{\hat{\rho}} = -\theta^2 [-k_2]^{-1} (\hat{C} - C). \end{cases} \quad (15)$$

This high-gain observer is independent of biomass measurements.

Adaptive control strategy

Generally speaking, a typical problem in the fed-batch bioprocess control is that of generating the substrate feed rate profile to optimize a performance criterion [6]. For our bioprocess, the main objective is to maintain a low level of the pollutant (substrate) concentration. This goal can be achieved through an optimal control, i.e. the calculation of a feeding rate optimal profile. This is unsatisfactory when the kinetics is imprecisely known. A possible suboptimal alternative is the adaptive control [6]. This well-known method [13] has a wide field of applications such as robotics [14, 15, 16], chemical and biochemical processes [6, 7] and so on.

Next, an exact linearizing control law is obtained for the wastewater treatment process. Then, an adaptive version of this controller is implemented, considering that X and μ are unknown, and by using the estimators

described before.

The achievement of the exact linearizing control law for the model (4) is done in a classical three steps strategy (see [6, 13, 17]). The control goal is that the substrate concentration $y(t) = \xi_2(t) = S(t)$ to track the desired substrate trajectory $y^*(t) = S^*(t)$, with the feeding rate as control action: $u(t) = F_{in}(t)$. First, from (3) one obtains a bioprocess input-output model

$$\dot{y} = \dot{S} = \dot{\xi}_2 = -k_1\mu(y)\xi_1 + (u/V)(S_{in} - y). \quad (16)$$

Second, we consider a stable and linear reference model for the tracking error $y^* - y$

$$(\dot{y}^* - \dot{y}) + \lambda(y^* - y) = 0, \lambda > 0. \quad (17)$$

Third, the linearizing control law is obtained by calculus of u such that (16) has the same behavior as (17)

$$u(t) = V \cdot (k_1\mu(y)\xi_1 + \lambda(y^* - y)) / (S_{in} - y) \quad (18)$$

with the reference $y^* = const$.

The exact linearizing control (18) can ensure the achievement of control goal only if the concentration $\xi_1 = X$ is on-line measurable and the specific growth rate is known. Contrarily, if the estimations provided by the estimators are used in the exact linearizing control law, adaptive versions of the nonlinear law are obtained. For example, if the estimations $\hat{\rho}(t) = \hat{\mu}(t)$ provided by (12) are used in the control law (18), an adaptive version of this law is obtained as follows

$$u(t) = V \cdot (k_1\hat{\mu}X + \lambda(y^* - y)) / (S_{in} - y). \quad (19)$$

When X cannot be measured, the asymptotic observer (13), (14) can be used, and another adaptive controller is

$$u(t) = V \cdot (k_1\hat{\mu}X_{est} + \lambda(y^* - y)) / (S_{in} - y). \quad (20)$$

The entire adaptive control algorithm consists of equations (12)-(14) and (20). Regarding the stability and convergence properties of the controlled system, these are widely discussed for bioprocesses in [2, 6].

Remark 3. A simpler version of the nonlinear adaptive control law can be obtained for those practical situations when the endogenous respiration kinetic coefficient b is negligible. Then, the reaction rate $\hat{\rho}(t) = \hat{\phi}(t)$ is the unknown kinetic parameter, which is estimated by using the observer (15), and subsequently used in the following version of adaptive controller (20)

$$u(t) = V \cdot (k_1\hat{\phi} + \lambda(y^* - y)) / (S_{in} - y). \quad (21)$$

As it can be seen, for this version of the adaptive control law the measurements or the estimates of biomass concentration are no more needed.

Simulation results

In order to analyze the behavior and the performances of the proposed estimation and control strategies, extensive

simulations were performed. The fed-batch bioprocess has been simulated by numerical integration of the basic model equations (3), considering μ of the form (5), and the following process parameters [4, 10]: $\mu^* = 0.1916h^{-1}$, $K_S = 60mg4CP/l$, $K_I = 3.753mg4CP/l$, $k_1 = 3.7mg4CP/mgVSS$, $k_2 = 1.0363mgDO/mgVSS$, $b = 0.0059h^{-1}$, $K_La = 16.8h^{-1}$, $C_S = 600mg/l$.

The bioprocess behavior was analyzed assuming that the influent substrate and dissolved oxygen concentrations act as perturbations of sinusoidal form (with a period of two hours and an amplitude between 2600 and 4400 mg/l), and of rectangular form (with a period of two hours and an amplitude between 45 and 75 mg/l), respectively. The next simulation scenarios were taken into consideration:

i) The exact linearizing control law (18) was implemented for the process (3), with $\lambda = 5$. The closed loop system was tested for a step profile of substrate reference. Fig. 1 presents the evolution of the substrate concentration versus the reference profile. This case is a kind of benchmark, an ideal situation, because all states and parameters are considered to be known. The time profile of the control input is shown in Fig. 2. The controlled bioprocess has a very good evolution, which can be improved for larger values of λ .

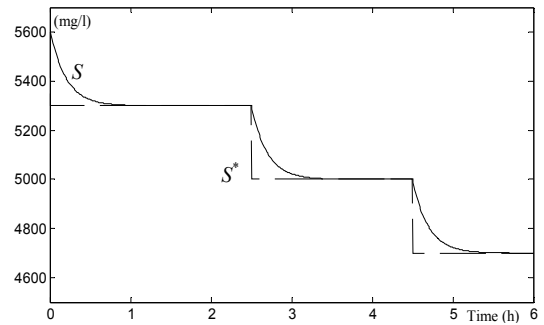


Fig. 1. Evolution of the output versus reference – the exact linearizing control case

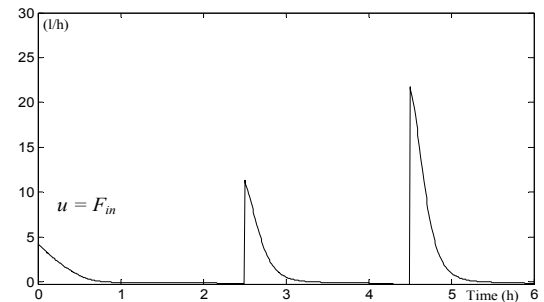


Fig. 2. Time profile of the control input – the exact linearizing control case

ii) The nonlinear adaptive control law (20) was implemented. Thus, the specific growth rate and the biomass concentration are considered as unknown, and consequently the high-gain observer (12) and the asymptotic observer (13), (14) were used. The goal of high gain observer (12) is to reconstitute the time evolution of μ from the measurements of C and the estimates of X

provided by the observer (13), (14). The “true” values of the specific rate (5) are used only for the simulation of measured data from the process. The tuning parameter was set to $\theta = 25$. To test the robustness of observers to noisy measurements, the measurements of C are vitiated by an additive Gaussian noise (zero mean and amplitude 1% of the free noise values). Fig. 3 depicts the time evolution of the dissolved oxygen concentration in both cases (with and without noise). The biomass concentration and the estimations provided by the asymptotic observer are shown in Fig. 4. To compare the performance of the proposed high gain algorithm with another estimation technique, the observer-based estimator (OBE) designed in [4] was also implemented. The estimation results obtained with both estimators are presented in Fig. 5. It can be seen that the high-gain observer behaves slightly better than the OBE.

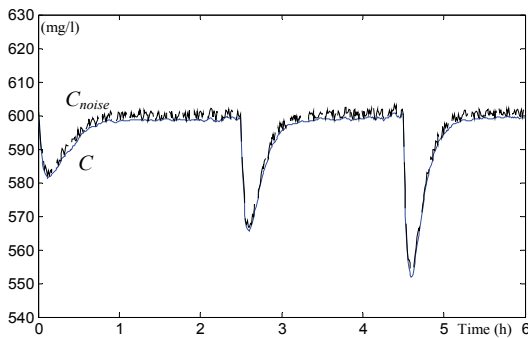


Fig. 3. The evolution of dissolved oxygen concentration – free noise measurements and noisy measurements

The estimates (biomass concentration – asymptotic observer, and specific growth rate provided by the high gain observer) are used in the adaptive control law (20).

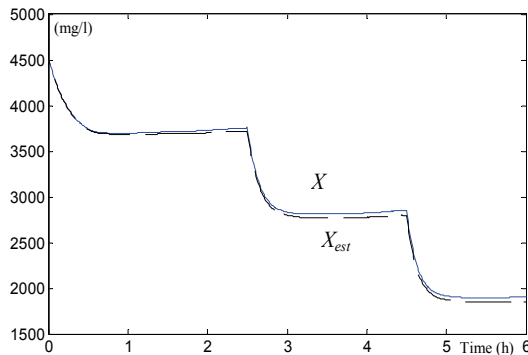


Fig. 4. Time profiles of the biomass concentration versus its estimate – adaptive control case

Fig. 6 shows the profile of the output versus reference in this second simulation scenario. Finally, Fig. 7 presents the profile of the control action in the adaptive control simulation case. The estimations of the specific growth rate are a little bit sensible to the noisy measurements, but the output seems to be more robust from this point of view. Overall, it can be observed the good behavior of the adaptive controller, despite the partially knowledge of kinetics, the unavailability of X measurements, and the action of noisy measurements. Several supplementary simulations were conducted for various values of noise, and for different values of tuning parameters. As a

conclusion, the estimation precision can be increased as much as possible by using larger values of θ .

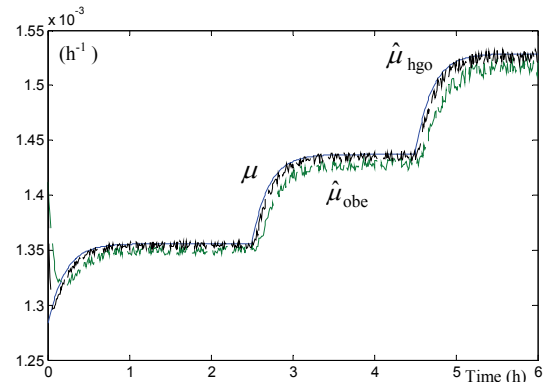


Fig. 5. Estimation results – the “true” specific growth rate (blue line) and estimations provided by the high-gain observer (hgo – black line) and by the observer-based estimator (obe – green line)

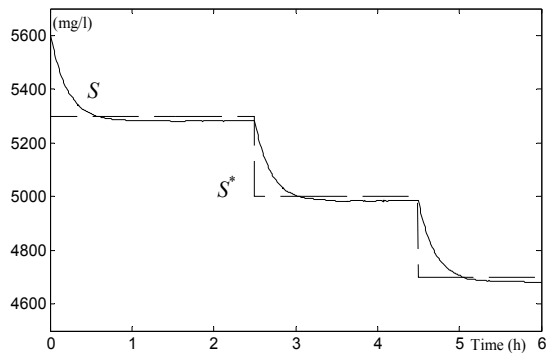


Fig. 6. Time evolution of the output (substrate concentration) versus reference – adaptive control case

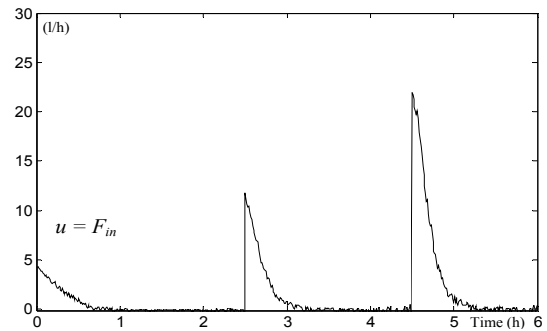


Fig. 7. Time profile of the control input – adaptive control case

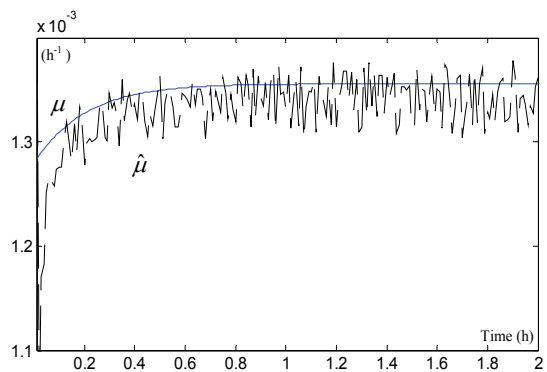


Fig. 8. Estimated growth rate (hgo) for large noise values (zoom)

This scenario is valid for the case of free noise measurements. Contrarily, the high-gain estimator becomes noise sensitive (see for example Fig. 8 – zoom for an additive noise of 5% amplitude of the free noise values, $\theta = 50$), and consequently the estimations cannot be used for the implementation of the adaptive control law.

Conclusions

The obtained results show a good behavior of the adaptive controlled wastewater treatment bioprocess inside a Sequencing Batch Reactor. The nonlinear control strategy is a combination of a high-gain estimator for the unknown kinetics, an asymptotic observer for the estimation of unavailable biomass concentration, and of an exact linearizing control law.

The behavior of the controlled system was tested using realistic simulations, considering some parametric disturbances and noisy measurements. The control goal, i.e. the preservation of a low level of pollutant concentration, is accomplished despite these disturbances. The results can be improved for the free-noise case by increase of the tuning parameter of high-gain estimator. However, for noisy measurements the observer can become noise sensitive. The proposed adaptive control scheme is quite simple, because only two tuning parameters were used, one for estimator and one for the linearizing controller.

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This work approaches the on-line estimation and adaptive control of a wastewater treatment process, which takes place inside a bioreactor. This bioprocess is highly nonlinear, the available state measurements are lack and moreover the reaction kinetics is not perfectly known. The kinetic parameters are estimated by using high-gain nonlinear observers and the unavailable states are reconstructed by using an asymptotic state observer. The control goal is to keep a low level of pollutant concentration. An adaptive control law is designed by combining a linearizing controller with the nonlinear observers. Numerical simulations are included to test the performances of the proposed algorithms. Ill. 8, bibl. 17 (in English; abstracts in English and Lithuanian).

M. Roman, D. Selişteanu. Netiesinis realaus laiko nuotekų valymo bioprocso vertinimas ir adaptyvusis valdymas // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2012. – Nr. 1(117). – P. 23–28.

Pateikti realaus laiko nuotekų valymo proceso, vykstančio bioreaktoriuje, vertinimas ir adaptyvusis valdymas. Šis procesas yra netiesinis, naudojami būsenų matavimai turi trūkumų ir reakcijos kinetika nėra tiksliai žinoma. Kinetiniai parametrai įvertinami naudojant didelio stiprinimo netiesinius stebiklius, o nesamos būsenos yra rekonstruojamos naudojant asimptotinį būsenų stebiklį. Valdymo tikslas – palaikyti žemą teršalų koncentracijos lygį. Adaptyviojo valdymo taisyklė yra sudaryta kombinuojant tiesinimo valdiklį su netiesiniais stebikliais. Siūlomų algoritmų veiksmingumui nustatyti buvo atliktos skaitmeninės imitacijos. Il. 8, bibl. 17 (anglų kalba; santraukos anglų ir lietuvių k.).