

ON-LINE MONITORING OF A BIOLOGICAL PROCESS FOR WASTEWATER TREATMENT

MONITOREO EN LINEA DE UN PROCESO BIOLOGICO PARA TRATAMIENTO DE AGUAS RESIDUALES

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Abstract

In this work, the problem of on-line monitoring of the pollutant concentrations is tackled in two biological reactors in series for industrial and municipal wastewater treatment. For this purpose, a software sensor is designed for on-line estimation of the pollutant concentrations, mainly for ammonia and biodegradable substrate. First, a reduced process model is developed with approximated parameters. Then the software sensor, consisting of a model-based state estimator to infer the (unmeasured) concentrations, is constructed based on the reduced process model and considering only on-line measurements of dissolved oxygen and nitrate concentrations. The software sensor performance is tested by comparison with the dynamic behavior of a detailed simulated plant (in a commercial software: GPS-X[®], Hydromantis) that represents the "experimental" process, obtaining good estimated concentrations. The simulated plant was previously tuned with experimental data collected from the *Tecnocasic* (Cagliari, Italy), which collects industrial and municipal wastewater.

Keywords: estimators, detectability, state estimation, biological reactors.

Resumen

En este trabajo se aborda el problema de monitoreo en línea de las concentraciones de contaminantes en dos reactores biológicos en serie para el tratamiento de aguas residuales industriales y municipales. Para este propósito, se diseña un software sensor para la estimación de las concentraciones contaminantes, principalmente de amoníaco y sustrato biodegradable. Primero, se desarrolla un modelo reducido del proceso con parámetros aproximados. Luego el software sensor, que consiste de un estimador de estados basado en un modelo para inferir las concentraciones (no medibles), se construye con base en el modelo reducido y considerando solo mediciones en línea de las concentraciones de oxígeno disuelto y de nitrato. El desempeño del software sensor es probado mediante la comparación con el comportamiento dinámico de una planta simulada detalladamente (en un software comercial: GPS-X[®], Hydromantis), que representa el proceso "experimental", obteniéndose buenos estimados de las concentraciones. La planta simulada fue previamente ajustada con datos experimentales recolectados de la planta *Tecnocasic* (Cagliari, Italia), la cual recolecta aguas residuales industriales y municipales.

Palabras clave: estimadores, detectabilidad, estimación de estados, reactores biológicos.

1. Introduction

During the last decade the interest in removal of pollutant compounds from wastewater has risen due to increasing attention for many reasons: regulation constraints, environment, water reuse, etc. Biological wastewater treatment is an essential operation for the processing of liquid waste, where the main objectives are

the degradation of the organic pollutant compounds and the removal of nutrients such as nitrogen that can damage the ecosystem. In particular, the activated sludge process is the most widely used process for biological treatment of municipal or industrial wastewater.

Working on the monitoring and control of biological wastewater treatment processes raises a number of very challenging problems

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as (Shimizu, 1996): the lack of reliable sensors, the significant model uncertainty, and the nonlinear time-varying nature of the system. Indeed, if a number of on-line sensors providing state information are today available at the industrial scale, they may be still very expensive and their maintenance is usually time consuming. To overcome these difficulties, the notion of software sensors has been introduced in the early eighties. In fact, the software sensors simply consist of observers or detectors designed to estimate unmeasured states from the available on-line measurements (Dochain *et al.*, 1997; Gauthier and Kupka, 1994; De Asís and Filho, 2000). Having an important advantage since software sensors can be constructed based on a simple model with uncertain inputs and parameters (Stephanopoulos and San, 1984). Recently, several studies have been reported concerning the software sensor design for the biological wastewater treatment. Many of those studies are related to the single aerobic process (to mention: Dochain and Pauss, 1988; Aubrun *et al.*, 2001; Bernand *et al.*, 2001), but few works have tackled the (anoxic-aerobic) alternating process (Zhao and Kümmel, 1995; Lukasse *et al.*, 1999; Larose and Jorgensen, 2001; Gomez-Quintero and Queinnec, 2001). The majority of the reported works are based on the extended Kalman filter (EKF) algorithm, while asymptotic observers are seldom used (Bernand *et al.*, 2001; Larose and Jorgensen, 2001). Moreover, the software sensor performances have been tested by simulation and few of them correspond to real (experimental) applications.

The EKF (Jazwinski, 1970) is by far the most widely used state estimation technique. Its construction is systematic, but it presents several drawbacks, for instance: it does not have a systematic tuning procedure, there is not convergence criterion, it is sensitive to changes in the initial state conditions and in the tuning parameters, and covariance matrices have to be well settled to get good

performance. On the other hand, the geometric system approach has presented high-gain low-order estimation designs with convergence criteria coupled to rather simple tuning schemes (Isidori, 1995; Ciccarella *et al.*, 1993), including the cases of complete and partial observability (Alvarez and Lopez, 1999); and these designs have been successfully tested in various simulated and experimental chemical processes (Van Dootting *et al.*, 1992; Soroush *et al.*, 1997). Thus the question is whether these low-order nonlinear estimation designs can be applied (instead of the EKF) to solve the software sensor problem in an alternating anoxic-aerobic process for wastewater treatment.

In this work, the on-line monitoring of a biological process (an alternating anoxic-aerobic process) for the wastewater treatment is tackled, by means of a software sensor designed for the estimation of the pollutant concentrations. First, a reduced process model is developed with approximated parameters, based on concepts widely accepted in the wastewater community. Then the software sensor, consisting of a nonlinear geometric state estimator (Alvarez and Lopez, 1999), is constructed to infer the (unmeasured) biodegradable substrate and ammonia concentrations, based on the reduced process model and considering on-line measurements of dissolved oxygen and nitrate concentrations. Here it is important to mention that detectability conditions are proved and stated with physical meaning, in contrast to reported works for biological processes. Finally, the software sensor performance is tested by comparison with the dynamic behavior of a detailed simulated plant (in a commercial software: GPS-X[®], Hydromantis), that represents the “experimental” process, obtaining good estimated concentrations and highlighting the ability of using simple and approximated models together with few on-line measurements. In particular the simulated plant was previously tuned with experimental

data collected from the *Tecnocasic* plant (Cagliari, Italy), which collects industrial and municipal wastewater, and its biological treatment is carried out by the alternating activated sludge process.

2. Biological process

2.1 Process description

In general, wastewater treatment includes as a first step a mechanical and chemical treatment to remove floating and settleable solids, then a biological treatment with activated sludge for removal of nitrogen, phosphorus and other organic pollutants, and after that other operations such as sludge treatment and water chemical treatment.

Here only the continuous alternating activated sludge process (AASP) is considered for the biological wastewater treatment with the main purpose of nitrogen removal. In general, the AASP employs aerated, tubular, well mixed or a series of well-mixed reactors to accommodate the biological process. In particular we are considering a sequence of two well-mixed reactors, Fig. 1. The water recycling from one reactor to another is common feature of

combined stabilization-denitrification networks, so that a combined oxidation and reduction in total nitrogen content is done by two different conditions: (i) an anoxic zone that favors the pre-denitrification step, and (ii) an aerobic zone that favors the nitrification one. Afterward the reactor network effluent is generally fed into a settler to separate the stream into the clean effluent and sludge. The settled sludge is partly recycled to the first reactor (return activated sludge, RAS) and a fraction is purged (waste activated sludge, WAS) from the recycle line to compensate for the increase in biomass concentration from biomass growth during the biodegradation process.

The global process is considered isothermal (around 20°C), and both anoxic (with low aeration for mixing purposes) and aerobic (with high aeration for reaction and mixing purposes) zones are controlled by the aeration supply by turbines. The AASP is very sensitive to input-flow oscillations, operation conditions and biomass evolution (Maria *et al.*, 2000). So that, the process characterization requires extensive off-on line investigations under a wide range of operation conditions.

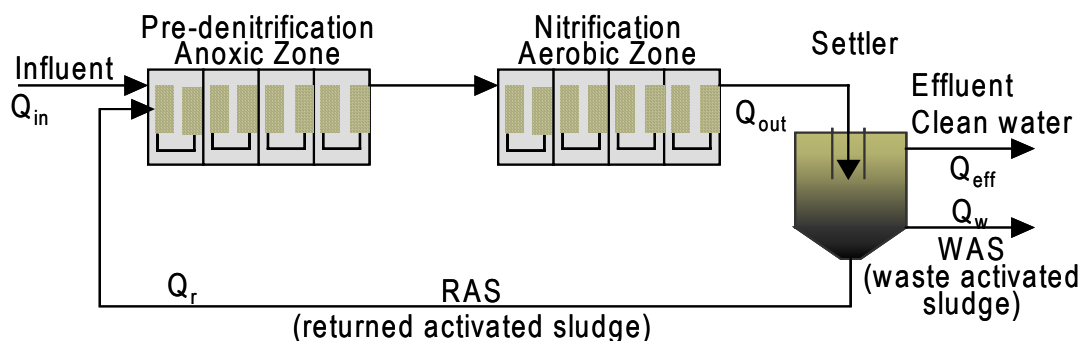


Fig. 1. Biological process (alternating activated sludge process).

2.2 Process model

In particular, as mentioned in the introduction, we are considering a real case study: the *Tecnocasic* plant (Cagliari, Italy), which collects industrial and municipal wastewater, and its treatment is done by the AASP as described previously. Its complete characterization has been done previously, and a detailed model with identified parameters was previously tuned using real experimental data taken from the *Tecnocasic* plant (Mulas, 2001).

The characterization was done by simulations in the GPS-X[®] (a commercial software of Hydromantis), using the two-step-mantis model (Technical reference manual, 2001) which corresponds to the so-called IAWQ Activated Sludge Model No. 1 (Henze *et al.*, 1987) with two modifications: (a) the nitrification is modeled by a two-step process (the conversion of ammonia to nitrite by the nitrosomona bacteria and the conversion of nitrite to nitrate by the nitrobacters), and (b) the hydrolysis of rapidly biodegradable substrate is included. This complete and complex model that will be referred as the “actual process model” consists of 18 state variables (particle and soluble concentrations) for each anoxic and aerobic reactor, so that the process is modeled with 36 ordinary differential equations, including 15 reaction rates and 30 model parameters. The actual process model simulation is included in order to show afterwards the advantages of using simple models together with the available measurements, since a great problem for having an exact model is the parameter identification which strongly changes for each waste and biomass type (Maria *et al.*, 2000).

Since we are interested in having estimates of soluble concentrations (which are not modified by the settler, but only the particle concentrations that are not calculated here), a reduced model proposed by Gomez-

Quintero *et al.* (2000) is considered. Differently from the plant model, this one consists of 8 state variables: dissolved ($S_{O_2}^p, S_{O_2}^n$), nitrate ($S_{NO_3}^p, S_{NO_3}^n$), ammonia ($S_{NH_4}^p, S_{NH_4}^n$) and biodegradable substrate (S_S^p, S_S^n) concentrations for each reactor zone (p and n denote pre-denitrification and nitrification, respectively); including only 5 lumped reaction rates with 11 model parameters. The *reduced model* for the pre-denitrification reactor is given as follows:

$$\begin{aligned} \frac{dS_{NO_3}^p}{dt} &= \frac{Q_{in}}{V} S_{NO_3}^{in} + \frac{Q_r}{V} S_{NO_3}^n - \frac{Q_{out}}{V} S_{NO_3}^p \\ &\quad - \left(\frac{1-Y_H}{2.86Y_H} \right) r_1^p + r_2^p := f_1 \end{aligned} \quad (1a)$$

$$\begin{aligned} \frac{dS_{O_2}^p}{dt} &= \frac{Q_r}{V} S_{O_2}^n - \frac{Q_{out}}{V} S_{O_2}^p + K_{La} (S_{OST} - S_{O_2}^p) \\ &\quad - 4.57r_2^p - \left(\frac{1-Y_H}{Y_H} \right) r_3^p := f_2 \end{aligned} \quad (1b)$$

$$\begin{aligned} \frac{dS_{NH_4}^p}{dt} &= \frac{Q_{in}}{V} S_{NH_4}^{in} + \frac{Q_r}{V} S_{NH_4}^n - \frac{Q_{out}}{V} S_{NH_4}^p \\ &\quad - i_{XB} (r_1^p + r_3^p) - r_2^p + \alpha_3 := f_3 \end{aligned} \quad (1c)$$

$$\begin{aligned} \frac{dS_S^p}{dt} &= \frac{Q_{in}}{V} S_S^{in} + \frac{Q_r}{V} S_S^n - \frac{Q_{out}}{V} S_S^p \\ &\quad - \frac{1}{Y_H} (r_1^p + r_3^p) + r_4^p + r_5^p := f_4 \end{aligned} \quad (1d)$$

and for the nitrification reactor:

$$\begin{aligned} \frac{dS_{NO_3}^n}{dt} &= \frac{Q_{out}}{V} (S_{NO_3}^p - S_{NO_3}^n) \\ &\quad - \left(\frac{1-Y_H}{2.86Y_H} \right) r_1^n + r_2^n := f_5 \end{aligned} \quad (1e)$$

$$\frac{dS_{O2}^n}{dt} = \frac{Q_{out}}{V} (S_{O2}^p - S_{O2}^n) + K_{La}^n (S_{OST} - S_{O2}^n) - 4.57 r_2^n - \left(\frac{1 - Y_H}{Y_H} \right) r_3^n := f_6 \quad (1f)$$

$$\frac{dS_{NH4}^n}{dt} = \frac{Q_{out}}{V} (S_{NH4}^p - S_{NH4}^n) - i_{XB} (r_1^n + r_3^n) - r_2^n + \alpha_3 := f_7 \quad (1g)$$

$$\frac{dS_S^n}{dt} = \frac{Q_{out}}{V} (S_S^p - S_S^n) - \frac{1}{Y_H} (r_1^n + r_3^n) + r_4^n + r_5^n := f_8 \quad (1h)$$

The lumped reaction rates are given by (p/n means either p or n):

$$r_1^{p/n} = \alpha_1 \left(\frac{S_{NO3}^{p/n}}{K_{NO3} + S_{NO3}^{p/n}} \right) \left(\frac{K_{O2,H}}{K_{O2,H} + S_{O2}^{p/n}} \right) S_s^{p/n} \quad (2a)$$

$$r_2^{p/n} = \alpha_2 \left(\frac{S_{NH4}^{p/n}}{K_{NH4} + S_{NH4}^{p/n}} \right) \left(\frac{S_{O2}^{p/n}}{K_{O2,A} + S_{O2}^{p/n}} \right) \quad (2b)$$

$$r_3^{p/n} = \alpha_1 \left(\frac{S_{O2}^{p/n}}{K_{O2,H} + S_{O2}^{p/n}} \right) S_s^{p/n} \quad (2c)$$

$$r_4^{p/n} = \alpha_4 \eta_H \left(\frac{S_{NO3}^{p/n}}{K_{NO3} + S_{NO3}^{p/n}} \right) \left(\frac{K_{O2,H}}{K_{O2,H} + S_{O2}^{p/n}} \right) \quad (2d)$$

$$r_5^{p/n} = \alpha_4 \left(\frac{S_{O2}^{p/n}}{K_{O2,H} + S_{O2}^{p/n}} \right) \quad (2e)$$

The reduced model parameters (α_i) are obtained as follows:

$$\alpha_1 = k_2 \mu_H \gamma X_{BH}, \quad \alpha_2 = \frac{\mu_A X_{BA}}{Y_A} \quad (3a)$$

$$\alpha_3 = K_A X_{BH} S_{ND}, \quad \alpha_4 = k_1 k_h X_{BH} \quad (3b)$$

Where all parameters μ_H , μ_A , η_H , γ , i_{XB} , Y_H , Y_A , k_1 , k_2 , k_A , K_A , $K_{O2,H}$, K_{O2} , k_A , K_{NO3} , and K_{NH4} (see Nomenclature for definitions) were identified using the software GPS-X[®].

2.3 Test motion

As it was aforementioned, the actual process model was tuned before using experimental data collected in the real plant, thus here only the result motion is presented, as it will be referred as the *actual process motion*. This motion, Fig. 2, is obtained with an operation condition that was set around the mean value $\{\bar{S}_{NO3}^{in}, \bar{S}_{NH4}^{in}, \bar{S}_S^{in}, \bar{Q}_{in}, \bar{Q}_r, \bar{Q}_w, \bar{V}\} \approx \{0.0 \text{ g/m}^3, 16.25 \text{ g N/m}^3, 118.3 \text{ g COD/m}^3, 6200 \text{ m}^3/\text{d}, 7800 \text{ m}^3/\text{d}, 560 \text{ m}^3/\text{d}, 2000 \text{ m}^3\}$ with some disturbances. The identified parameters for the reduced model, Eq. 3, are given in Table 1. In Fig. 2 the actual process motion as well as the reduced model motion are shown, where it can be seen that the reduced model gives the motion tendency but with significant offsets due to the errors in the model assumptions and parameter identification. With this simulation, it can be stated one of the tasks that the on-line monitoring approach should do. Specifically in the present work we propose a software sensor (equivalently to a state estimator based on the reduced model and some measurements) to give good inference of the modeling errors in order to reach the actual process motion.

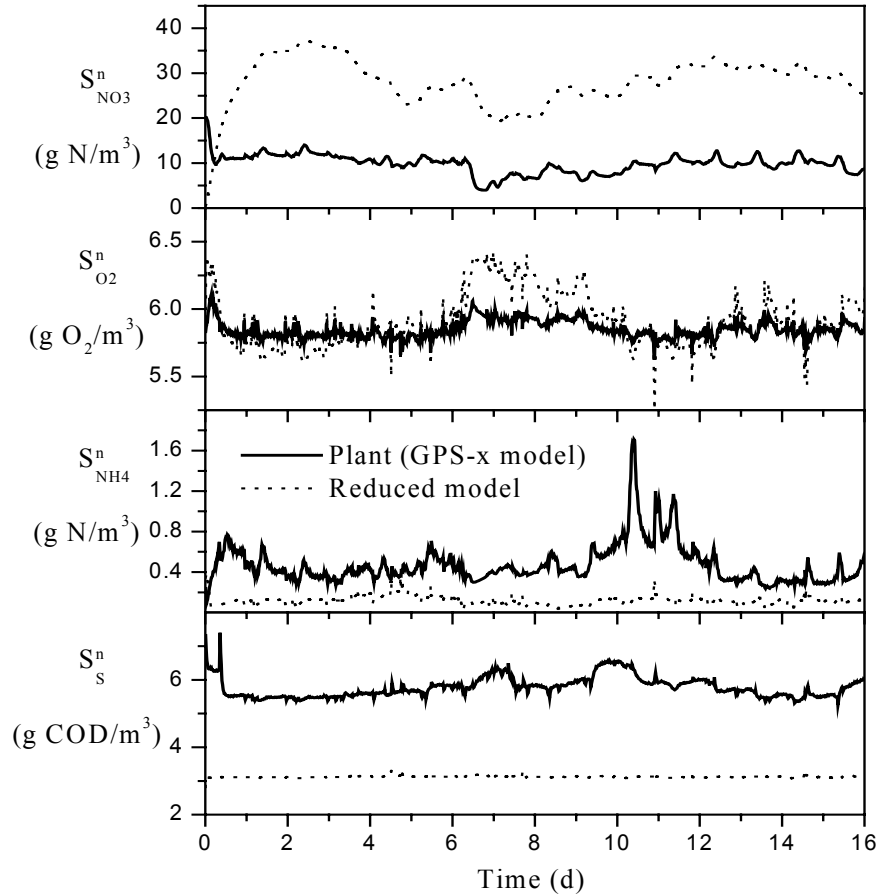


Fig. 2. Time evolution of the nitrification reactor: actual reactor (—) and reduced model (····) motions.

Table 1. Model parameters

Parameter (p)	Value
Y_H	0.7
i_{XB}	$0.086 \text{ g N (g COD)}^{-1}$
$K_{O2,H}$	$0.2 \text{ g O}_2 \text{ m}^{-3}$
$K_{O2,A}$	$0.23 \text{ g O}_2 \text{ m}^{-3}$
K_{NO3}	0.1 g N m^{-3}
K_{NH4}	$0.8 \text{ g NH}_3\text{-N m}^{-3}$
η_H	0.4
α_1	163.9 d^{-1}
α_2	$224.63 \text{ g m}^{-3} \text{ d}^{-1}$
α_3	$92.12 \text{ g m}^{-3} \text{ d}^{-1}$
α_4	$739.74 \text{ g m}^{-3} \text{ d}^{-1}$

2.4 On-line monitoring problem

In our study case, the on-line monitoring problem consists on designing a software sensor for estimating mainly the ammonia and biodegradable substrate concentrations in the biological process exit, from available measurements of dissolved oxygen and ammonia concentrations in the exit flow.

Let us start by writing the estimation problem in state-space notation, considering the next state vector:

$$x = [x_1, \dots, x_8]^T = [S_{NO_3}^p, S_{O_2}^p, S_{NH_4}^p, S_S^p, S_{NO_3}^n, S_{O_2}^n, S_{NH_4}^n, S_S^n]^T \quad (4a)$$

exogenous input vector

$$d = [d_1, \dots, d_6]^T = [S_{NO_3}^{in}, S_{NH_4}^{in}, S_S^{in}, Q_{in}/V, Q_r/V, Q_w/V]^T \quad (4b)$$

model parameter vector

$$p = [p_1, \dots, p_{12}]^T = [Y_H, i_{XB}, K_{O_2,H}, K_{O_2,A}, K_{NO_3}, K_{NH_4}, \eta_H, \alpha_1, \alpha_2, \alpha_3, \alpha_4]^T \quad (4c)$$

and measured output vector

$$y = [y_1, y_2]^T = [S_{NO_3}^n, S_{O_2}^n]^T \quad (4d)$$

The reduced model, Eq. 1, can be rewritten as

$$\dot{x} = f(x, d, p) \quad (5a)$$

$$y = h(x) \quad (5b)$$

The state x ($x \in X$), the input d ($d \in D$), and the parameter p ($p \in P$) take values in the sets X , D and P , respectively, and are compact (i.e., bounded and closed) due to physical and practical considerations. The maps $f(x, d, p)$ and $h(x)$ are respectively the right side of Eq. 1 and Eq. 4d, and are sufficiently smooth (differentiable) in their respective domains. So that the software sensor will consist of a state estimator based on the reduced model Eq. 5a and the two measurements taken in the aerobic zone Eq. 5b, and it should be robust to have tolerance to the modeling error and to the uncertain inputs and measured outputs.

3. Software sensor design

For this purpose, the design is based on the geometric nonlinear estimation methodology developed in Alvarez and Lopez (1999) and Lopez (2000), which has a

systematic construction, with a robust convergence criterion connected to the convergence rate, and with a simple tuning procedure. It is worth of mention that our aim is the development of a software sensor for our case study by using this low-order nonlinear estimation design (instead of the EKF), so that the estimator details can be found in the aforementioned works. Next the detectability analysis, the estimator construction and tuning are presented for our specific case study.

3.1 Estimation structure

According to Alvarez and Lopez (1999), the motion $x(t)$ of the biological process, Eqs. 5, can be completely observable with observability indices $(\kappa_1, \kappa_2) = (4, 4)$ for the two measured outputs, Eq. 5b, proposed here, however the observability property would be weak (i.e. with an observability matrix ill-conditioned due to the third time-derivatives required). Taking as a point of departure the results on the effect of the estimation structure in the estimator functioning given in Lopez and Alvarez (2004), the biological process can be detectable (i.e. partial observable) with several estimation structures (i.e. combination of the observability indices and of the observable-unobservable state partition). Moreover, between all of the possible estimation structures, the one that keeps the tradeoff between robustness and performance is the corresponding one with observability indices

$$(\kappa_1, \kappa_2) = (2, 2) \quad (6)$$

and with the state partition (x_I and x_{II} are the observable and unobservable states, respectively)

$$x_I = [x_5, x_6, x_7, x_8]^T, \quad x_{II} = [x_1, x_2, x_3, x_4]^T \quad (7)$$

The detectability property follows from the assessment of the two following conditions [along the reactor motion $x(t)$]:

- (i) The map $\phi(x, d, p)$, Eq. 8, has to be invertible for x_I .
- (ii) The motions of the unobservable dynamics $x_{II}(t)$ have to be stable.

Where the map ϕ is given by the measured outputs and some of their time-derivatives:

$$\begin{aligned} \phi(x, d, p) &= [y_1, \dot{y}_1, y_2, \dot{y}_2]^T \\ &= [x_5, f_5(x, d, p), x_6, f_6(x, d, p)]^T \end{aligned} \quad (8)$$

To verify that the plant motion is detectable for all time, the two previous conditions were verified. First, given the matrix Q (called *observability matrix*)

$$Q = \frac{\partial \phi}{\partial x_I} \quad (9)$$

the invertibility condition [condition (i)] is equivalent to verify that $\text{Rank}[Q] = \kappa_1 + \kappa_2 = 4$, or else, $\det[Q] \neq 0$ for all time. The corresponding determinant expression is as follows

$$\begin{aligned} \det[Q] &= \frac{\alpha_1 \alpha_2 K_{NH4}}{(K_{NH4} + S_{NH4}^n)^2} \left(\frac{1 - Y_H}{Y_H} \right) \left(\frac{1}{K_{O2,H} + S_{O2}^n} \right) \\ &\quad \left(\frac{S_{O2}^n}{K_{O2,A} + S_{O2}^n} \right) \left[\frac{K_{O2,H} S_{No3}^n}{1.598 (K_{No3} + S_{No3}^n)} + S_{O2}^n \right] > 0 \end{aligned} \quad (10)$$

In fact this condition is always met since all model parameters are positive, $S_{No3}^n > 0$ and $S_{O2}^n > 0$ (i.e., nitrate and oxygen concentrations in the nitrification reactor which is an aerobic zone). Moreover, it was also evaluated numerically as can be seen in Fig. 3a, showing that $\det[Q] > 0$ for all time.

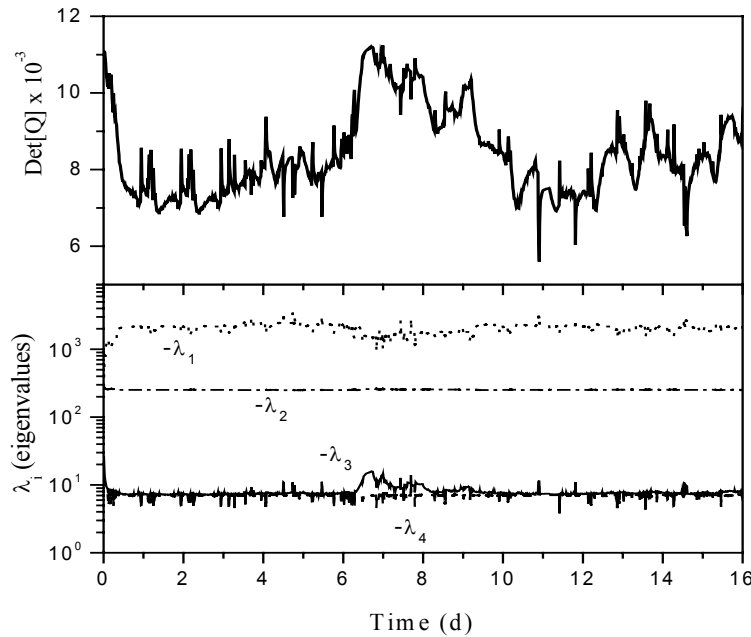


Fig. 3. (a) Determinant of the observability matrix, and (b) eigenvalues of the unobservable dynamics, along the actual reactor motion.

The assessment of the stability condition [condition (ii)] is equivalent to verify that the unobservable dynamics given by:

$$\dot{x}_1 = f_1(x_1, x_2, x_3, x_4, \bar{x}_5, \bar{d}, p) \quad (11a)$$

$$\dot{x}_2 = f_2(x_2, x_3, x_4, \bar{x}_6, \bar{d}, p) \quad (11b)$$

$$\dot{x}_3 = f_3(x_1, x_2, x_3, x_4, \bar{x}_7, \bar{d}, p) \quad (11c)$$

$$\dot{x}_4 = f_4(x_1, x_2, x_4, \bar{x}_8, \bar{d}, p) \quad (11d)$$

are stable, considering \bar{x}_5 , \bar{x}_6 , \bar{x}_7 , \bar{x}_8 and \bar{d} as nominal known motions. These equations are stable if the eigenvalues of its linear system have strictly negative real part. This is verified also numerically along the reactor motion and is shown in Fig. 3b, concluding that the dynamics are stable.

As the two detectability conditions are met, therefore the reactor motion is detectable, and a state estimator can be implemented. Furthermore, this estimation structure can be applied to any AASP as both detectability conditions are always met.

3.2 Nonlinear state estimator

Considering the previous state partition, Eq. 7, the reactor, Eq. 5, can be rewritten as

$$\dot{x}_I = f_I(x_I, x_{II}, d, p) \quad (12a)$$

$$\dot{x}_{II} = f_{II}(x_I, x_{II}, d, p) \quad (12b)$$

$$y = h(x_I) \quad (12c)$$

The construction of the geometric estimator (Luenberger-like high-gain) follows from a straightforward consequence

of the detectability property, according to the following expression (see Theorem 1 in Alvarez and Lopez, 1999). So that the estimator for our case is given by:

$$\begin{aligned} \dot{\hat{x}}_I &= f_I(\hat{x}_I, \hat{x}_{II}, d, p) + \\ Q^{-1}(\hat{x}_I, \hat{x}_{II}, d, p) K_o [y - h(\hat{x}_I)] \end{aligned} \quad (13a)$$

$$\dot{\hat{x}}_{II} = f_{II}(\hat{x}_I, \hat{x}_{II}, d, p) \quad (13b)$$

$$\hat{y} = h(\hat{x}_I) \quad (13c)$$

Where Q^{-1} is the inverse of the observability matrix, Eq. 9, and K_o is the gain matrix. It can be seen that the observable part Eq. 13a, of the estimator has two terms: (i) the first one corresponds to a predictor given by the model, and (ii) the second one corresponds to a corrector driven by the measurement error. While the unobservable part, Eq. 13b, only has the predictor term given by the model.

Regarding to the gain matrix, this one should be chosen such that the estimation error dynamics are stable. Some strategies for the estimator tuning are also given in Alvarez and Lopez (1999) and Lopez (2000). According to this, the gains can be calculated as follows

$$K_o = \begin{bmatrix} k_{11} & 0 \\ k_{12} & 0 \\ 0 & k_{21} \\ 0 & k_{22} \end{bmatrix}, \quad \begin{aligned} k_{11} &= 2\zeta\omega_i \\ k_{12} &= (\omega_i)^2 \end{aligned} \quad (14)$$

where ζ is the damping factor, which can be set according the literature (Stephanopoulos, 1984) as $\zeta = 0.71$ in order to have a response with moderate oscillations. While ω_i is the characteristic frequency, which can be selected such that the estimator response is

faster than the natural reactor response. For this purpose, first we calculated the residence time ($\theta = 0.143$ d), then to obtain an estimator response faster, we selected the estimator characteristic time as $\omega_i > 10 / \theta$. Meaning that a good initial guess can be $\omega_i = 70$ d⁻¹. In fact after some trials, the final tuning values were set as $\omega_1 = \omega_2 = \omega_3 = 150$ d⁻¹ (≈ 20 times faster than the natural dynamics).

The convergence properties of the geometric nonlinear estimation methodology (Alvarez and Lopez, 1999; Lopez, 2000) ensure the asymptotic convergence of the state estimator for the biological process. In fact, the convergence criterion is in function of the fulfillment of the previous detectability conditions and of the high gain tuning.

4. Implementation results

The main objective is the on-line monitoring of the pollutant and biomass concentrations of the clean effluent. It is important to keep in mind that the settler does not modify these soluble concentrations, so that the soluble concentrations at the nitrification reactor exit are the same of the clean water in the settler exit, Fig. 1. Thus, the results for the nitrification (aerobic) reactor exit are shown in Fig. 4. As it was mentioned in Section 3.1, all concentrations in the pre-denitrification reactor are unobservable states (x_{II}) and those ones in the nitrification reactor are observable states (x_I). Meaning that the unobservable states are estimated only with the model [i.e., the predictor term in, Eq. 13b, so that their convergence rate is not controlled, while the observable ones are estimated using the model and a predictor term, Eq. 13a, that is dependent on the gain matrix K_o and the unobservable states. Therefore, the rate convergence of the estimated concentrations in the nitrification reactor is function of: (a) the tuning, which has been done as fast as possible to get a fast convergence, and (b) the

slow convergence rate of the unobservable concentrations in the pre-denitrification reactor, involving an estimation delay. According to this, as it can be seen in Fig. 4, there is almost exact converge for the measured states (S_{NO3}^n, S_{O2}^n). The small offsets in these two states are due to the frequent excitations especially in the dissolved oxygen concentration as a consequence of the disturbances in the feed concentrations and flows. In fact, the two main concentrations of interest in the process exit are the ammonia S_{NH4}^n and the biodegradable substrate S_S^n , which show very good estimates since the estimator follows the tendency motion and the offsets are still acceptable in comparison with the measuring error of a concentration instrument. So we can say that the software sensor is reliable, in spite of using a reduced model that by itself (i.e. without the corrections terms added in the estimator) has large modeling errors as was shown before in Fig. 2.

Conclusions

It has been shown how to reduce a state estimation problem for the on-line monitoring of a biological process used in the wastewater treatment. This study highlights the ability of using a software sensor based upon a reduced model (with large model parameter errors) and considering only two on-line measurements (dissolved oxygen and nitrate concentrations). The software sensor performance was validated with a plant motion obtained from previous detailed plant characterization, showing that not always the use of complex models is the best way to obtain good process representation for monitoring and control purposes. The implementation of a software sensor gives promising guidelines to tackle in the future the problems of optimization and real time control of wastewater treatment plants.

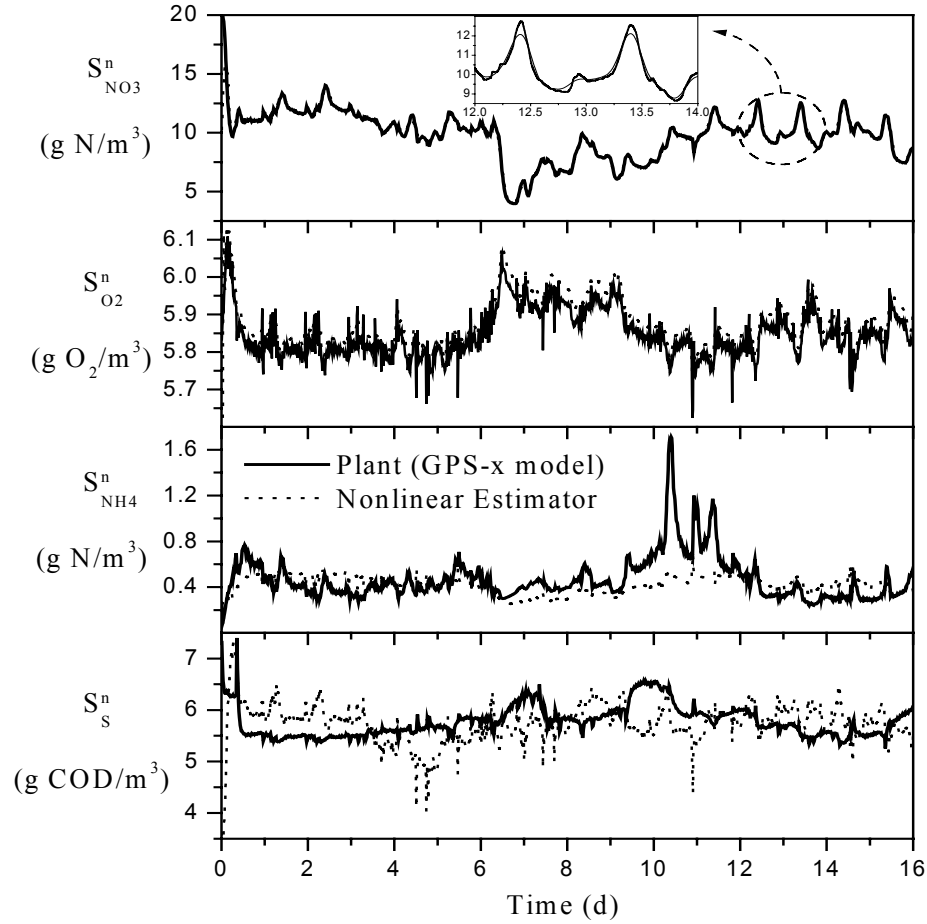


Fig. 4. Software sensor performance (·····) in comparison with the actual motion (————) for the nitrification reactor.

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Nomenclature

Latin variables

d	Exogenous input
f	Model map
i_{XB}	Mass N/mass COD in biomass [-]
K_o	Observability matrix gain
k_{La}	Oxygen mass transfer coefficient [d^{-1}]
k_i	i -th Identified model parameter, $i = 1, 2$ [-]

k_h	Maximum specific hydrolysis rate [d^{-1}]
K_A	Ammonification rate [$m^3(g\ COD\ d)^{-1}$]
$K_{O2,H}$	Aerobic oxygen half saturation coefficient [$g\ O_2\ m^{-3}$]
$K_{O2,A}$	Aerobic/anoxic oxygen half saturation coefficient [$g\ O_2\ m^{-3}$]
K_{NO3}	Nitrate half-saturation coefficient [$g\ N\ m^{-3}$]
K_{NH4}	Ammonia half saturation coefficient [$g\ N\ m^{-3}$]
p	Model parameter
Q	Observability matrix
Q_n	Flow rate, $n = in, out, r, w$ [$m^3\ d^{-1}$]
r_i	i -th Reaction rate, $1 \leq i \leq 5$ [$g\ m^{-3}\ d^{-1}$]
S_{NO3}	Nitrate concentration [$g\ N\ m^{-3}$]
S_{O2}	Dissolved oxygen concentration [$g\ O_2\ m^{-3}$]

S_{NH4}	Ammonia concentration [g N m ⁻³]
S_{ND}	Average soluble biodegradable organic nitrogen concentration [g N m ⁻³]
S_S	Biodegradable substrate concentration [g COD m ⁻³]
S_{OST}	Dissolved oxygen saturation concentration [g O ₂ m ⁻³]
V	Reactor volume [m ³]
x	Process state
X_{BA}	Average active autotrophic biomass concentration [g COD m ⁻³]
X_{BH}	Average active heterotrophic biomass concentration [g COD m ⁻³]
y	Measured output
Y_A	Autotrophic yield [-]
Y_H	Heterotrophic yield [-]

Greek variables

α_1	1 st Reduced model parameter [d ⁻¹]
α_i	i -th Reduced model parameter, $i = 2, 3, 4$ [g m ⁻³ d ⁻¹]
γ	Identified model parameter [g ⁻¹ m ³]
η_H	Correction factor for anoxic hydrolysis [-]
ϕ	Observable map
κ_i	i -th Observability index, $i = 1, 2$
μ_A	Maximum specific autotrophic growth rate [d ⁻¹]
μ_H	Maximum specific heterotrophic growth rate [d ⁻¹]
ζ	Damping factor [-]
ω_i	Characteristic frequency, $i = 1, 2$ [d ⁻¹]

Subscripts

in	influent
r	RAS
w	WAS
out	reactor exit
eff	(clean) effluent
I	observable partition
II	unobservable partition

Superscripts

p	pre-denitrification
n	nitrification
\wedge	estimated

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