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Coupled robust observer to estimate the glucose at the input of a biohydrogen production reactor

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Abstract: In this article a coupled observer to estimate the glucose concentration at the input of a hydrogen production reactor is proposed. The observer developed consists of a Luenberger observer coupled to a super-twisting observer. The Luenberger observer is used to estimate the concentrations inside the reactor. The super-twisting observer uses the precedent estimations to estimate the glucose at the reactor input. Convergence of the observer is discussed and results demonstrate the feasibility of the strategy proposed.

Keywords: Biohydrogen production, robust estimation, super-twisting observer, Luenberger observer, control H_∞.

1. INTRODUCTION

Biological production of hydrogen (biohydrogen), using (micro) organisms, is an area of technology development that offers the potential production of usable hydrogen from a variety of renewable resources. Biological systems provide a wide range of approaches to generate hydrogen, and include direct biophotolysis, indirect biophotolysis, photo-fermentations, and dark-fermentation, Levin et al. (2004).

Once a biological system to produce hydrogen has been developed, the operational conditions have to be optimized in order to achieve a desirable process performance.

In this context, Ramirez et al. (2012) proposed a real-time optimization strategy to maximize the hydrogen productivity of a fermentation reactor. The process productivity, depending on the organic loading rate (OLR), was defined as objective function. The OLR depends on both, the flow rate (Q_{in}) and the substrate concentration (Glu_{in}) at the reactor input. Q_{in} was selected as the optimization variable while Glu_{in} was maintained constant along the process operation. Nevertheless, Glu_{in} is in reality a bounded perturbation varying along the time which must be known in order to correctly maximize the hydrogen productivity. Since measure the glucose concentration at the reactor input on-line is not practical, it must be estimated.

The problem of estimating unknown inputs in biotechnological processes has been addressed before in several works. For instance, Moreno and Dochain (2013) proposed a discontinuous observer able to estimate in finite time both unmeasured states and the unknown input of a SISO nonlinear second order system. The only requirements are the observability of both the states and the unknown input, and that the unknown input is a uniformly Lipschitz time function. This strategy was tested in a simple biotechnological model. Aceves-Lara et al. (2007) addressed the problem of estimating simultaneously the states and the input concentrations of an acidogenic process used for biohydrogen production. The input and states concentrations were estimated using a state transformation and an asymptotic observer. In this work, we propose an alternative strategy to estimate the unmeasured input of a bioreactor for hydrogen production by coupling a Luenberger observer to a super-twisting observer.

The hydrogen production reactor has two inputs, Glu_{in} (an uncontrolled input) and Q_{in} (a controlled input). On the other hand, the total gas flow rate (Q_{gas}) and the hydrogen fraction ($\%H_2$) at the reactor output are measured. Using these measurements, the hydrogen flow rate ($q_{H2,gas}$) can be calculated.

As shown in figure 1, the observer consists in a Luenberger observer followed by a super-twisting observer. By measuring $q_{H2,gas}$, the Luenberger observer estimates the glucose and the biomass concentrations in the reactor. Then, the super-twisting observer uses these estimations to estimate the glucose concentration at the reactor input.

The article is organized as follows: section 2 presents the model of the anaerobic hydrogen production reactor used to develop the coupled observer. In section 3 the super-twisting observer to estimate the input glucose is presented. Since the super-twisting observer needs the glucose and the biomass concentrations inside the reactor to be implemented, in section 4 a robust Luenberger observer is developed to estimate them. In section 5

results are presented and discussed. Finally, section 6 is devoted to conclusions.

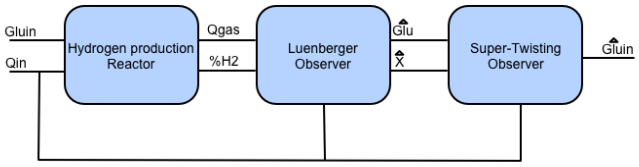

Fig. 1. Block diagram of the observation system.

2. MODEL OF THE HYDROGEN PRODUCTION REACTOR

The anaerobic hydrogen production reactor considered in this work is modeled, as proposed in Aceves-Lara et al. (2008), by the following set of ordinary differential equations (ODE):

$$\begin{bmatrix} \dot{Glu} \\ \dot{Ace} \\ \dot{Pro} \\ \dot{Bu} \\ \dot{X} \\ \dot{CO_2} \\ \dot{H_2} \end{bmatrix} = Kr - D \begin{bmatrix} Glu - Glu_{in} \\ Ace \\ Pro \\ Bu \\ X \\ CO_2 \\ H_2 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ q_{CO_2,gas} \\ q_{H_2,gas} \end{bmatrix} \quad (1)$$

where Glu, Ace, Pro, Bu, X, CO_2 and H_2 represent the concentrations in gL^{-1} of glucose, acetate, propionate, butyrate, biomass, carbon dioxide and hydrogen, respectively, in the liquid phase. The vector r describes the kinetics of the involved biological reactions (in $gL^{-1}d^{-1}$), D is the dilution rate (d^{-1}) and $q_{CO_2,gas}$ and $q_{H_2,gas}$ the gas flow rates of carbon dioxide and hydrogen expressed in $gL^{-1}d^{-1}$, respectively. Finally, $K \in \mathbb{R}^{7\times 2}$ represents the matrix of pseudo-stoichiometric coefficients.

The reaction pathway is described by two reactions occurring in parallel. Thus, the vector r is composed of the specific glucose uptake rate multiplied by the biomass concentration in the reactor:

$$r = \begin{bmatrix} \dfrac{\mu_{max1} Glu}{K_{Glu1} + Glu} \\ \dfrac{\mu_{max2} Glu}{K_{Glu2} + Glu} \end{bmatrix} X$$

Furthermore, the differential equations for the gas phase with constant gas volume are:

$$\frac{dCO_{2,gas}}{dt} = -\frac{CO_{2,gas} Q_{gas}}{V_{gas}} + \rho_{CO_2} \frac{V}{V_{gas}} \quad (2)$$

$$\frac{dH_{2,gas}}{dt} = -\frac{H_{2,gas} Q_{gas}}{V_{gas}} + \rho_{H_2} \frac{V}{V_{gas}} \quad (3)$$

with:

$$Q_{gas} = \frac{RT_{amb}}{P_{atm} - p_{vap,H_2O}} V \left(\frac{\rho_{H_2}}{M_{H_2}} + \rho_{CO_2} \right) \quad (4)$$

$$\rho_{H_2} = k_L a_{H_2} (H_2 - M_{H_2} K_{H,H_2} p_{H_2,gas}) \quad (5)$$

$$p_{H_2,gas} = \frac{H_{2,gas} RT_{reac}}{M_{H_2}} \quad (6)$$

$$\rho_{CO_2} = k_L a_{CO_2} (CO_2 - K_{H,CO_2} p_{CO_2,gas}) \quad (7)$$

$$p_{CO_2,gas} = CO_{2,gas} RT_{reac} \quad (8)$$

where $CO_{2,gas}$ and $H_{2,gas}$ are, respectively, the carbon dioxide concentration, in $molL^{-1}$, and the hydrogen concentration, in gL^{-1}, in the gas phase.

As shown in equation (4), the total gas flow at the reactor output is the sum of the hydrogen gas flow plus the carbon dioxide gas flow. The carbon dioxide and the hydrogen gas flow rates are calculated by considering the transfer of the gas out from the liquid phase to the gas phase. The carbon dioxide and the hydrogen concentrations at the liquid-gas interface in equilibrium are calculated by considering the Henry law. The pressure of each gas component can be calculated using the ideal gas law for the two gases.

In the following sections, the values of the constants used in the reactor model are taken from Aceves-Lara et al. (2008).

3. ESTIMATION OF THE GLUCOSE AT THE REACTOR INPUT

The glucose dynamics is modeled by:

$$\begin{aligned} \dot{Glu} &= k_{11} r_1 + k_{12} r_2 - D(Glu - Glu_{in}) \\ \dot{Glu} &= DGlu_{in} + h(Glu, X) \end{aligned}$$

where $h(Glu, X) = k_{11} r_1 + k_{12} r_2 - DGlu$. $DGlu_{in}$ is unknown but it is an absolutely continuous function of time, its dynamics can therefore be modeled as:

$$\frac{d(DGlu_{in})}{dt} = \delta_2(t)$$

Thus, the dynamics of Glu and $DGlu_{in}$ is modeled by the following ODE system:

$$\begin{aligned} \dot{Glu} &= DGlu_{in} + h + \delta_1(t); \;\; |\delta_1| \leq c_1, \; c_1 > 0 \\ (\dot{DGlu_{in}}) &= \delta_2(t); \;\; |\delta_2| \leq c_2, \; c_2 > 0 \end{aligned} \quad (9)$$

Note that $\delta_2(t)$ captures the uncertainties about $DGlu_{in}$ while $\delta_1(t)$ captures the uncertainties about r, Glu and X.

A super-twisting observer is then proposed to estimate Glu_{in} as:

$$\begin{aligned} \dot{\hat{Glu}} &= (D\hat{Glu_{in}}) + h(Glu, X) + \gamma_1 \phi_1(\epsilon_1) \\ (\dot{D\hat{Glu_{in}}}) &= \gamma_2 \phi_2(\epsilon_1) \end{aligned} \quad (10)$$

where:

$$\epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \end{bmatrix} = \begin{bmatrix} Glu - \hat{Glu} \\ DGlu_{in} - (D\hat{Glu}_{in}) \end{bmatrix}$$

$$\phi_1(\epsilon_1) = |\epsilon_1|^{1/2}\text{sign}(\epsilon_1)$$

$$\phi_2(\epsilon_1) = \frac{1}{2}\text{sign}(\epsilon_1)$$

Fridman et al. (2011) propose the following linear matrix inequality (LMI) to calculate the observer gain $\Gamma = [\gamma_1 \ \gamma_2]^T$:

$$\begin{bmatrix} \Lambda^T\Omega_1 + \Omega_1\Lambda + \varepsilon I_2 + \Psi & \Omega_1\Upsilon \\ \Upsilon^T\Omega_1 & -\Theta \end{bmatrix} \leq 0 \tag{11}$$

where Θ and Ψ are defined as:

$$\Theta = \begin{bmatrix} \theta_1 & 0 \\ 0 & \theta_2 \end{bmatrix}, \ \Psi = (\theta_1 g_1^2 + \theta_2 g_2^2)\Xi\Xi^T$$

Besides $\Lambda = \Lambda_\epsilon - \Gamma\Xi$ and the constant matrices are defined as:

$$\Lambda_\epsilon = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \ \Upsilon = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \ \Xi = [\,1 \ 0\,]$$

Using the classical circle criterium, a didactic statement can be found in Khalil (2002), the LMI (11) will be satisfied if and only if the H_∞ norm of the transfer function $G_\epsilon(s) = \Xi(sI - \Lambda)^{-1}\Upsilon$ is less than $1/\max(g_1, g_2)$.

Therefore, the following matrix inequality will be satisfied as well, Scherer and Weiland (2004):

$$\begin{bmatrix} \Lambda^T\Omega_1 + \Omega_1\Lambda + \Xi\Xi^T & \Omega_1\Upsilon \\ \Upsilon^T\Omega_1 & -\alpha^2 I_2 \end{bmatrix} \leq 0 \tag{12}$$

where:

$$\alpha < \frac{1}{\max(g_1, g_2)} \tag{13}$$

An observer gain Γ with the objective to decrease the influence of the uncertainties δ_1 and δ_2 on the estimation error ϵ, may be computed by minimizing the H_∞ norm of the transfer function G_ϵ, as proposed in the optimization problem (14), Scherer and Weiland (2004), Fridman et al. (2011).

In (14) $\alpha \in \mathbb{R}$, $\Omega_1 \in \mathbb{R}^{2\times 2}$, $\Omega_2 \in \mathbb{R}^{2\times 1}$, $\Theta \in \mathbb{R}^{2\times 2}$, $\varepsilon \in \mathbb{R}$, $g_1|\phi_1(\epsilon_1)| = c_1$ and $g_2|\phi_2(\epsilon_1)| = c_2$. The observer gain, solution of the optimization problem (14), is then calculated as $\Gamma = \Omega_1^{-1}\Omega_2$ and $\|G_\epsilon\|_\infty = \alpha$.

In order to implement the super-twisting observer (10) the current concentrations of glucose and biomass inside the reactor are needed. Therefore, in the following section a robust Luenberger observer is developed to estimate the concentrations inside the biohydrogen production reactor by measuring the hydrogen flow rate at the reactor output.

4. ESTIMATION OF THE CONCENTRATIONS INSIDE THE REACTOR

Let the state vector $x \in \mathbb{R}^4$ be defined as:

$$x = \begin{bmatrix} Glu \\ X \\ H_2 \\ H_{2,gas} \end{bmatrix}$$

Let us define in addition $u = Q_{in}$ as the controlled input and $w = Glu_{in}$ as a disturbance.

A reduced nonlinear system can be defined as:

$$\dot{x}(t) = f(x, u, w) \tag{15}$$

By linearizing the non-linear model (15) around an operating point (x^*, u^*, w^*), a reduced linear state space model is obtained as:

$$\dot{\bar{x}}(t) = A\bar{x}(t) + B_u\bar{u}(t) + B_w\bar{w}(t) \tag{16}$$

where:

- A is the Jacobian matrix $J_f(x)|_{(x^*,u^*,w^*)}$.
- B_u is the Jacobian matrix $J_f(u)|_{(x^*,u^*,w^*)}$.
- B_w is the Jacobian matrix $J_f(w)|_{(x^*,u^*,w^*)}$.
- $\bar{x}(t) = x(t) - x^*$.
- $\bar{u}(t) = u(t) - u^*$.
- $\bar{w}(t) = w(t) - w^*$.

As mentioned in section 1, the output of the system is the hydrogen gas flow rate at the reactor output. Thus, according to equation (4) , the measured output is defined as:

$$y(t) = Cx(t) = \frac{RT_{amb}}{P_{atm} - p_{vap,H_2O}} V \left(\frac{\rho_{H_2}}{M_{H_2}}\right) \tag{17}$$

By regarding equations (5) and (6) it is easy to verify that matrix C takes the following form:

$$C = \begin{bmatrix} 0 & 0 & c_{H_2} & c_{H_{2,gas}} \end{bmatrix}$$

with:

$$c_{H_2} = \frac{RT_{amb}Vk_La_{H_2}}{(P_{atm} - p_{vap,H_2O})M_{H_2}}$$

$$c_{H_{2,gas}} = -\frac{R^2T_{amb}Vk_La_{H_2}K_{H,H_2}T_{reac}}{(P_{atm} - p_{vap,H_2O})M_{H_2}}$$

The measured output is defined in terms of $\bar{x}$ as:

$$\bar{y}(t) = y(t) - Cx^* = C\bar{x}(t) \tag{18}$$

The following Luenberger observer is proposed to estimate x without knowledge of w:

$$\dot{\hat{\bar{x}}}(t) = A\hat{\bar{x}}(t) + B_u\bar{u}(t) + L\left(\bar{y}(t) - \hat{\bar{y}}(t)\right) \tag{19}$$

$$\begin{aligned}
&\min_{\alpha,\Omega_1,\Omega_2,\varepsilon,\Theta} \alpha \\
&\text{such that:} \\
&\alpha > 0, \Omega_1 > 0, \varepsilon > 0, \Theta > 0 \\
&\max(g_1, g_2)\alpha < 1 \\
&\begin{bmatrix} \Omega_1\Lambda - \Omega_2\Xi + \Lambda^T\Omega_1 - \Xi\Omega_2^T + \Xi^T\Xi & \Omega_1\Upsilon & 0_2 \\ \Upsilon^T\Omega_1 & 0_2 & \alpha I_2 \\ 0_2 & \alpha I_2 & I_2 \end{bmatrix} < 0 \\
&\begin{bmatrix} \Omega_1\Lambda - \Omega_2\Xi + \Lambda^T\Omega_1 - \Xi\Omega_2^T + \varepsilon I_2 + \Psi & \Omega_1\Upsilon \\ \Upsilon^T\Omega_1 & -\Theta \end{bmatrix} \leq 0
\end{aligned} \tag{14}$$

Let $e = \bar{x} - \hat{\bar{x}}$ be the error between the real state vector $\bar{x}$ and the estimated state vector $\hat{\bar{x}}$. The transfer function from w to e is therefore given by:

$$G_{we}(s) = (sI - (A - LC))^{-1} B_w \tag{20}$$

An observer gain L with the objective to decrease the influence of the disturbance w on the estimation error e and accelerate its dynamics by placing its poles within the stability region $\mathcal{S}(d, r, \theta)$, proposed by Chilali and Gahinet (1996), and shown in figure 2, may be computed by minimizing the H_∞ norm of the transfer function G_{we} as proposed in the optimization problem (23).

In (23) $\gamma \in \mathbb{R}$, $W_1 \in \mathbb{R}^{4\times4}$ and $W_2 \in \mathbb{R}^{4\times2}$. As shown in figure 2, d is the distance between the origin and the vertical strip, r is the radius of the disk centered at the origin and θ is the angle (in radians) from the real axis to the strip defining the conic sector. The observer gain, solution of the optimization problem (23), is then calculated as $L = W_1^{-1}W_2$ and $\|G_{we}\|_\infty = \gamma$.

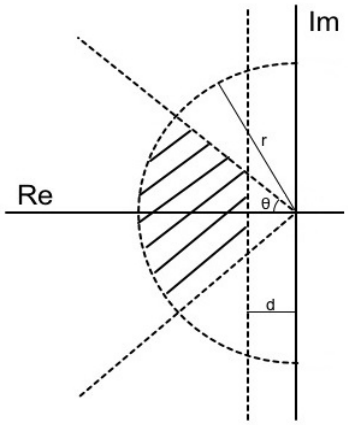

Fig. 2. Stability region $\mathcal{S}(d, r, \theta)$

By regarding equations (16) and (19) it is easy to verify that the dynamics of the estimation error e is given by:

$$\dot{e}(t) = (A - LC)e(t) + B_w w(t) \tag{21}$$

By solving the optimization problem (23) the eigenvalues of the dynamic matrix $A - LC$ in (21) are assigned in such a way that closed-loop stability is warranted and $e \to 0$ as $t \to \infty$ in spite of the disturbance w, Scherer and Weiland (2004), Chilali and Gahinet (1996). Therefore, the glucose concentration Glu and the biomass X inside the reactor asymptotically approach their true values.

On the other hand, by regarding equations (9) and (10) it is easy to verify that the dynamics of the estimation error ϵ is given by:

$$\dot{\epsilon}(t) = \Lambda\epsilon(t) + \Upsilon\Delta(t) - \Gamma_D\Phi(\epsilon_1) \tag{22}$$

with:

$$\Delta(t) = \begin{bmatrix} \delta_1(t) \\ \delta_2(t) \end{bmatrix},\ \Gamma_D = \begin{bmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{bmatrix},\ \Phi(\epsilon_1) = \begin{bmatrix} \phi_1(\epsilon_1) \\ \phi_2(\epsilon_1) \end{bmatrix}$$

If the optimization problem (14) has solution and the true values of both the glucose and the biomass inside the reactor are available, all trajectories of system (22) converge in finite time to the origin for all perturbations satisfying $|\delta_i| \leq g_i|\epsilon_1|$, for $g_i > 0$ and $i = 1, 2$, Fridman et al. (2011).

It must be point out that the dynamics of the Luenberger observer must be faster than the dynamics of the super-twisting observer in order to have available the true values of the glucose and the biomass inside the reactor to estimate the input glucose correctly.

5. RESULTS AND DISCUSSION

The complete observer to estimate the input glucose concentration is the Luenberger observer (19) coupled to the super-twisting observer (10). Optimization problems (14) and (23) were solved using the *SEDUMI* solver over the *YALMIP* toolbox in the *MATLAB* environment, Löfberg (2004).

By considering $|\delta_1| < 3.75$, $|\delta_2| < 3.5$ and $|\epsilon_1| < 2.5$ the following vector Γ was computed:

$$\Gamma = \begin{bmatrix} 0.8653 \\ 3.3543 \end{bmatrix} \times 10^6$$

On the other hand, the dynamics of the Luenberger observer was accelerated to converge to the real state faster than the super-twisting observer one, since the last needs the correct glucose and biomass concentrations inside the reactor to estimate correctly the input glucose. Thus, by placing the poles of the Luenberger observer within the stability region $\mathcal{S}(0, 7500, \pi/3)$ the following matrix L was computed:

$$\min_{\gamma, W_1, W_2} \gamma$$

such that:

$$\gamma > 0$$

$$W_1 > 0$$

$$\begin{bmatrix} W_1A - W_2C + A^TW_1 - C^TW_2^T + I_4 & W_1B_w & 0_{4,1} \\ B_w^TW_1 & 0 & \gamma \\ 0_{1,4} & \gamma & 1 \end{bmatrix} < 0 \tag{23}$$

$$W_1A - W_2C + A^TW_1 - C^TW_2^T + 2dW_1 < 0$$

$$\begin{bmatrix} -rW_1 & W_1A - W_2C \\ A^TW_1 - C^TW_2^T & -rW_1 \end{bmatrix} < 0$$

$$\begin{bmatrix} \sin(\theta)(W_1A - W_2C + A^TW_1 - C^TW_2^T) & \cos(\theta)(W_1A - W_2C - A^TW_1 + C^TW_2^T) \\ \cos(\theta)(A^TW_1 - C^TW_2^T - W_1A + W_2C) & \sin(\theta)(W_1A - W_2C + A^TW_1 - C^TW_2^T) \end{bmatrix} < 0$$

$$L = \begin{bmatrix} 182.82 \\ 1.49 \\ 0.10 \\ 0.04 \end{bmatrix}$$

The model of the hydrogen production reactor and the observers were simulated during 25 days in *MATLAB* considering a sample period $T = 4h$. In addition, the ODEs were solved using the *ode15s* solver. In order to demonstrate a proper convergence, the observer starts after five days from the process beginning.

Figure 3 shows in top the glucose concentration inside the reactor, in solid blue the 'real' concentration and in dashed red the estimated one. As can be observed in bottom, the estimation error remains very close to zero in the complete period of time.

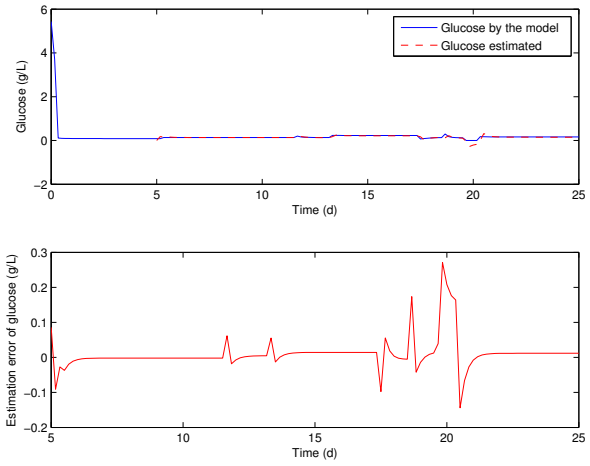

Fig. 3. Estimation of the glucose concentration inside the reactor. In top, in solid blue line the 'real' concentration and in dashed red line the estimated one. In bottom, the estimation error.

Figure 4 shows the biomass concentration inside the reactor. The biomass estimated converges after one day from the estimation beginning and then remains very close to the 'real' concentration, however, small transitions are presented when the biomass concentration changes. As can be regarded in bottom, the error concentration remains around zero in the complete period of time.

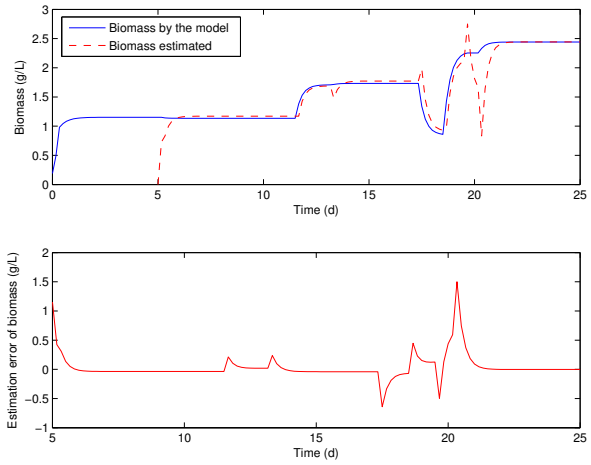

Fig. 4. Estimation of the biomass concentration inside the reactor. In top, in blue solid line the 'real' concentration and in red dashed line the estimated one. In bottom, the estimation error.

Once the glucose and the biomass concentrations inside the reactor have been estimated using the Luenberger observer (19), we are able to implement the super-twisting observer (10) to estimate the input glucose concentration. Nevertheless, the super-twisting observer estimates the dynamics of $DGlu_{in}$. Glu_{in} is therefore estimated as:

$$\hat{Glu}_{in} = \frac{(D\hat{G}lu_{in})}{D} = \frac{(D\hat{G}lu_{in})}{Q_{in}/V} = \frac{V(D\hat{G}lu_{in})}{Q_{in}}$$

Figure 5 shows the flow rate at the reactor input Q_{in} considered in this application.

In top of figure 6 the 'real' input glucose concentration (in solid blue) and the estimated one (in dashed red) are shown. As can be observed, the glucose concentration remains close to the 'real' one along the simulation, however, there exists a delay in the estimation when changes in the input glucose concentration are presented. In bottom, we can regard that the error estimation remains very close to zero for almost the complete period of time. Important estimation errors can be observed for the transition periods due to the delay mentioned before.

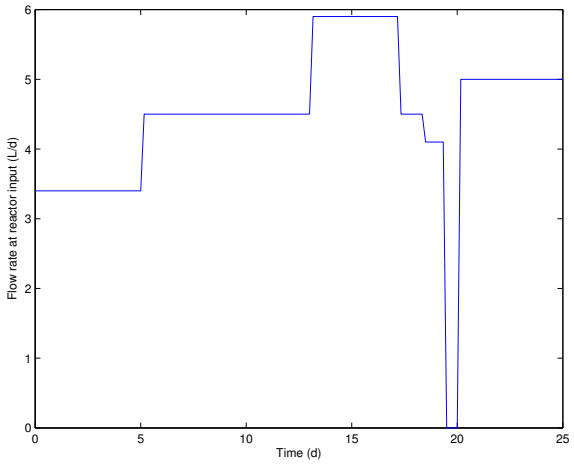

Fig. 5. Flow rate at the reactor input.

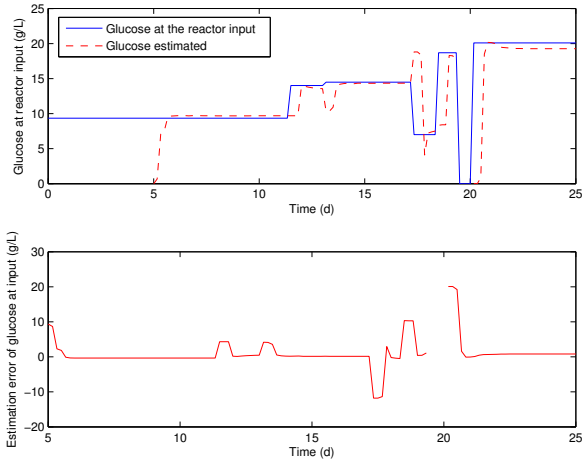

Fig. 6. Estimation of the input glucose concentration. In top, in solid blue line the 'real' concentration and in dashed red line the estimated one. In bottom, the estimation error.

6. CONCLUSIONS

In this work, a coupled observer to estimate the input glucose concentration in a bioreactor to produce hydrogen was developed. As the results showed in the previous section, the strategy proposed allows estimating the glucose at the reactor input very close to the 'real' values along the simulation period. Nevertheless, the convergence was not exact at all as we would expect due to the convergence discussion in section 4. This may be caused by the lack of an exact estimation of both the glucose and the biomass inside the reactor. It suggests that even if the Luenberger observer is robust, it does not minimize completely the influence of the disturbance on the error estimation, may be as consequence of the rank of the observability matrix $(rank(O) = 3)$. It mud be pointed out that the rank of subsystem x is superior $(rank(x) = 4)$.

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