Congreso Nacional de Control Automático 2013
Ensenada, Baja California, Mexico, Octubre 16-18, 2013

Coupled observer to estimate the substrate at the input of a hydrogen production reactor

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***Abstract*— This article presents a strategy to estimate the glucose concentration at the input of a hydrogen production reactor. The observer developed consists in a Luenberger observer coupled to a Super-Twisting one. The Luenberger observer uses the measured output of the process to estimate the glucose and the biomass concentrations inside the reactor. These estimations are taken by the Super-Twisting observer to estimate the glucose concentration at the reactor input. Results show that the estimated glucose at the reactor input follows correctly the real one and remains very close to it in most of the period of time considered.**
Keywords: Biohydrogen production, robust estimation, Super-Twisting observer, Luenberger observer, control H_2.

I. 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 [5].

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

In this context, in [7] the authors proposed a real-time optimization strategy to maximize the hydrogen productivity inside 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 solve the optimization problem to maximize the hydrogen productivity. Since measure the glucose concentration at the reactor input in real-time 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, in [10] an extended Luenberger observer has been proposed to estimate both the state and the unmeasured input for anaerobic wastewater treatment plants. In [8] the design of an observer for unknown inputs both constant and periodic (under the assumption of known frequency) is presented. In particular, in [2] the problem of estimating simultaneously the states and the input concentrations of an acidogenic process used for biohydrogen production is addressed. The input and states concentrations were estimated using a state transformation and an asymptotic observer. In this work, we propose an alternative strategy for estimating the unmeasured input of a biohydrogen production reactor by coupling a Luenberger observer to a Super-Twisting observer.

The hydrogen production reactor has two inputs, the substrate concentration Glu_{in} (an uncontrolled input) and the flow rate Q_{in} (a controlled input). On the other hand, the total gas flow rate (q_{Gas}) and the hydrogen fraction ($\%H_2$) at the output reactor are measured. Because the total gas at the reactor output is the sum of the hydrogen plus the carbon dioxide gases, the flow rates $q_{H_2,gas}$ and $q_{CO_2,gas}$ define the output of the system.

As shown in figure 1, the coupled observer consists in a Luenberger observer followed by a Super-Twisting one. By measuring both, the hydrogen and the carbon dioxide flow rates at the reactor output, the Luenberger observer estimates the glucose and the biomass concentrations into the reactor. Then, the Super-Twisting observer uses these estimations to estimate the glucose concentration at the reactor input.

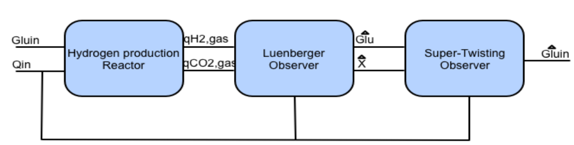

Fig. 1: Block diagram of the observation system.

The article is organized as follows: section II presents the model of the anaerobic hydrogen production reactor used to develop the coupled observer. In section III the Super-Twisting observer to estimate the glucose at the reactor input is presented. Since the Super-Twisting observer needs the glucose and the biomass concentrations inside the reactor to be implemented, in section IV a robust Luenberger observer is developed to estimate them. In section V results are presented and discussed. Finally, section VI is devoted to conclusions and future perspectives.

II. Model of the hydrogen production reactor

The anaerobic hydrogen production reactor considered in this work may be modeled, as proposed in [1], by the following set of ordinary differential equations (ODE):

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

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 $gL^{-1}d^{-1}$. 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:

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

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

$$\frac{dCO_{2,gas}}{dt} = -\frac{CO_{2,gas} q_{gas}}{V_{gas}} + \rho_{CO_2} \frac{V}{V_{gas}} \tag{2}$$

$$\frac{dH_{2,gas}}{dt} = -\frac{H_{2,gas} q_{gas}}{V_{gas}} + \rho_{H_2} \frac{V}{V_{gas}} \tag{3}$$

with:

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

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

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

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

$$p_{CO_2,gas} = CO_{2,gas} RT_{reac} \tag{8}$$

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 bar).

In the following sections, the values of the constants used in the reactor model are taken from [1].

III. Estimation of the glucose at the reactor input

The glucose dynamics is modeled by:

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

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:

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

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

A Super-Twisting observer is then proposed to estimate Glu_{in} as:

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

$$
\begin{array}{l}
\min_{\Omega_1,\Omega_2,\varepsilon,\Theta} trace(\Psi)\\
under\\
\Omega_1 > 0\\
\varepsilon > 0\\
\Theta > 0\\
\left[\begin{array}{cc} \Omega_1\Lambda - \Omega_2\Xi + \Lambda^T\Omega_1 - \Xi\Omega_2^T + \varepsilon I_2 + (\theta_1 g_1^2 + \theta_2 g_2^2)\Xi\Xi^T & \Omega_1\Upsilon \\ \Upsilon^T\Omega_1 & -\Theta \end{array}\right] \leq 0
\end{array} \tag{11}
$$

where:

$$
\epsilon = \left[\begin{array}{c} \epsilon_1 \\ \epsilon_2 \end{array}\right] = \left[\begin{array}{c} Glu - \hat{Glu} \\ DGlu_{in} - (\hat{DGlu_{in}}) \end{array}\right]
$$

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

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

An observer gain $\Gamma = [\gamma_1\ \gamma_2]^T$ 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 sector condition as proposed in the optimization problem (11) [4].

In (11) $\Omega_1 \in \mathbb{R}^{2\times 2}$, $\Omega_2 \in \mathbb{R}^{2\times 1}$, $\Theta \in \mathbb{R}^{2\times 2}$, $\varepsilon \in \mathbb{R}$, $g_1|\phi_1(\epsilon_1)| = c_1$ and $g_2|\phi_2(\epsilon_1)| = c_2$. Θ and Ψ are defined as:

$$
\Theta = \left[\begin{array}{cc} \theta_1 & 0 \\ 0 & \theta_2 \end{array}\right],\ \Psi = \left[\begin{array}{cc} -\Theta & 0_2 \\ 0_2 & (\theta_1 g_1^2 + \theta_2 g_2^2)\Xi\Xi^T \end{array}\right]
$$

Besides, the constant matrices are given as:

$$
\Lambda = \left[\begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array}\right],\ \Upsilon = \left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right],\ \Xi = \left[\begin{array}{cc} 1 & 0 \end{array}\right]
$$

The observer gain, solution of the optimization problem (11), is then calculated as $\Gamma = \Omega_1^{-1}\Omega_2$ [4].

In order to implement the Super-Twisting observer (10) the current concentrations of glucose and biomass are needed. Therefore, in the following section a Luenberger observer is developed to estimate the concentrations inside the biohydrogen production reactor by measuring both, the hydrogen and the carbon dioxide flows at the reactor output.

IV. Estimation of the concentrations inside the reactor

Let the state vector $x \in \mathbb{R}^6$ be defined as:

$$
x = \left[\begin{array}{c} Glu \\ X \\ CO_2 \\ H_2 \\ CO_{2,gas} \\ H_{2,gas} \end{array}\right]
$$

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:

$$
\dot{x}(t) = f(x, u, w) \tag{12}
$$

By linearizing the non-linear model (12) around an operating point (x^*, u^*, w^*), a reduced linear state space model is obtained as:

$$
\dot{\bar{x}}(t) = A\bar{x}(t) + B_u\bar{u}(t) + B_w\bar{w}(t) \tag{13}
$$

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 I, the output of the system is formed by both, the hydrogen and the carbon dioxide gas flows at the reactor output. The measured output is therefore defined as:

$$
y(t) = \left[\begin{array}{c} y_1(t) \\ y_2(t) \end{array}\right] = Cx(t) \tag{14}
$$

y_1 corresponds to the hydrogen flow rate and according to equation (4) is defined as:

$$
y_1 = \frac{RT_{amb}}{P_{atm} - p_{vap,H_2O}} V \left(\frac{\rho_{H_2}}{M_{H_2}}\right) \tag{15}
$$

y_2 corresponds to the carbon dioxide flow rate and according to equation (4) is defined as:

$$
y_2 = \frac{RT_{amb}}{P_{atm} - p_{vap,H_2O}} V \rho_{CO_2} \tag{16}
$$

By regarding equations (5)-(6) and (7)-(8) it is easy to verify that matrix C takes the following form:

$$
C = \left[\begin{array}{cccccc} 0 & 0 & 0 & c_{H_2} & 0 & c_{H_{2,gas}} \\ 0 & 0 & c_{CO_2} & 0 & c_{CO_{2,gas}} & 0 \end{array}\right]
$$

with:

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

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

$$c_{CO_2} = \frac{R T_{amb} V k_L a_{CO_2}}{P_{atm} - p_{vap,H_2O}}$$

$$c_{CO_{2,gas}} = \frac{R^2 T_{amb} V k_L a_{CO_2} K_{H,CO_2} T_{reac}}{P_{atm} - p_{vap,H_2O}}$$

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

$$\bar{y}(t) = y(t) - Cx^* = C\bar{x}(t) \tag{17}$$

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

$$\dot{\hat{\bar{x}}}(t) = A\hat{\bar{x}}(t) + B_u\bar{u}(t) + L\left(\bar{y}(t) - \hat{\bar{y}}(t)\right) \tag{18}$$

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:

$$G_{we}(s) = \left(sI - (A - LC)\right)^{-1} B_w \tag{19}$$

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 $\mathcal{S}(d, r, \theta)$, shown in figure 2, may be computed by minimizing the H_2 norm of the transfer function G_{we} as proposed in the optimization problem (22) [9], [3].

In (22) $W_1 \in \mathbb{R}^{6\times 6}$, $W_2 \in \mathbb{R}^{6\times 2}$ and $W_3 \in \mathbb{R}^{6\times 6}$. 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 (22), is then calculated as $L = W_1^{-1} W_2$ and $\|G_{we}\|_2 = trace(W_3)$ [9], [3].

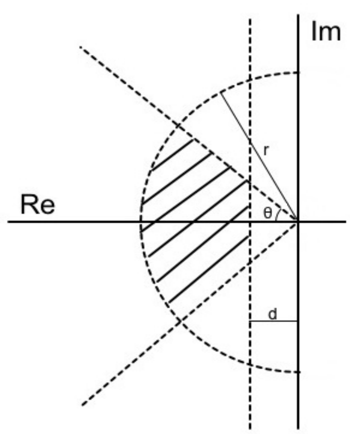

Fig. 2: Stability region $\mathcal{S}(d, r, \theta)$

By regarding equations (13) and (18) it is easy to verify that the dynamics of the estimation error e are given by:

$$\dot{e}(t) = (A - LC)e(t) + B_w w(t) \tag{20}$$

By solving the optimization problem (22) the eigenvalues of the dynamic matrix $A - LC$ in (20) are assigned in such a way that closed-loop stability is warranted and $e \rightarrow 0$ as $t \rightarrow \infty$ in despite of the disturbance w [9], [3]. Therefore, the glucose concentration Glu and the biomass X into 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:

$$\dot{\epsilon}(t) = \Lambda\epsilon(t) + \Upsilon\Delta(t) + \Gamma^T I_2 \Phi(\epsilon_1) \tag{21}$$

with:

$$\Delta(t) = \begin{bmatrix} \delta_1(t) \\ \delta_2(t) \end{bmatrix}, \; \Phi(\epsilon_1) = \begin{bmatrix} \phi_1(\epsilon_1) \\ \phi_2(\epsilon_1) \end{bmatrix}$$

If the optimization problem (11) has solution and the true values of both the glucose and the biomass into the reactor are available, all trajectories of system (21) converge in finite time to the origin for all perturbations satisfying $|\delta_i| \leq g_i|\epsilon_1|$, for $g_i > 0$ and $i = 1, 2$ [4].

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 into the reactor to estimate the glucose at the reactor input correctly.

V. Results and discussion

The complete observer to estimate the glucose concentration at the reactor input is the Luenberger observer (18) coupled to the Super-Twisting observer (10). Optimization problems (11) and (22) were solved using the *SEDUMI* solver over the *YALMIP* toolbox in the *MATLAB* environment [6].

By considering $|\delta_1| < 3.15$, $|\delta_2| < 2.575$ and $|\epsilon_1| < 2.5$ the following vector Γ was computed:

$$\Gamma = \begin{bmatrix} 0.2551 \\ 2.9953 \end{bmatrix} \times 10^6$$

On the other hand, the dynamics of the Luenberger observer were accelerated to converge to the real state faster than the Super-Twisting observer ones, since the last need the correct glucose and biomass concentrations to estimate correctly the glucose at the reactor input. Thus, by placing the poles of the Luenberger observer inside the stability region $\mathcal{S}(0, 1500, \pi/3)$ the following matrix L was computed:

$$
\begin{aligned}
&\min_{W_1,W_2,W_3} trace(W_3)\\
&under\\
&W_1 > 0\\
&\begin{bmatrix} W_1A - W_2C + A^TW_1 - C^TW_2^T + 2dW_1 & W_1B_w \\ B_w^TW_1 & -I \end{bmatrix} < 0\\
&\begin{bmatrix} -rW_1 & W_1A - W_2C \\ A^TW_1 - C^TW_2^T & -rW_1 \end{bmatrix} < 0\\
&\begin{bmatrix} sin(\theta)(W_1A - W_2C + A^TW_1 - C^TW_2^T) & cos(\theta)(W_1A - W_2C - A^TW_1 + C^TW_2^T) \\ cos(\theta)(A^TW_1 - C^TW_2^T - W_1A + W_2C) & sin(\theta)(W_1A - W_2C + A^TW_1 - C^TW_2^T) \end{bmatrix} < 0\\
&\begin{bmatrix} W_1 & I_6 \\ I_6 & W_3 \end{bmatrix} > 0
\end{aligned}
\qquad (22)
$$

$$
L = \begin{bmatrix} 13.8601 & 4.2975 \\ 0.2414 & 0.0760 \\ 0.0122 & -0.0240 \\ -0.0366 & 0.0066 \\ -0.0219 & 0.0247 \\ 0.0467 & -0.0526 \end{bmatrix}
$$

The model of the hydrogen production reactor and the observers were simulated during 25 days in *MATLAB* considering a sample period $T = 10min$. In addition, the ODEs were solved using the *ode15s* solver. In order to demonstrate a proper convergence, the observer starts after two days from the process beginning. Figure 3 shows the glucose concentration inside the reactor, in solid blue the 'real' concentration and in dashed black the estimated one. As can be observed, the estimations remain very close to the 'real' glucose concentration.

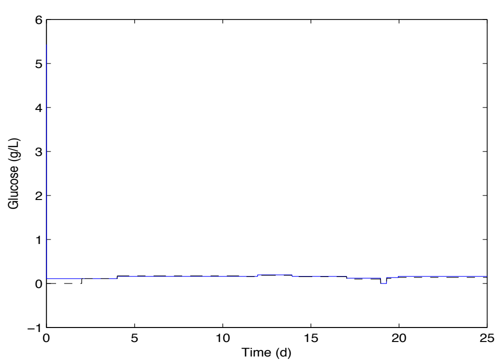

Fig. 3: Estimation of the glucose concentration inside the reactor. In blue solid line the 'real' concentration and in black dashed line the estimated one.

Figure 4 shows the biomass concentration inside the reactor. Biomass converge to the 'real' concentration between days 4 and 5, it remains very close to the 'real' concentration but between days 17 and 20 the disturbance is not correct rejected. It may be caused by the high variations in the glucose concentration at the reactor input (figure 6).

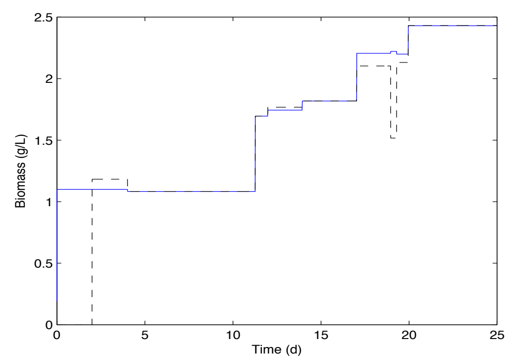

Fig. 4: Estimation of the biomass concentration inside the reactor. In blue solid line the 'real' concentration and in black dashed line the estimated one.

Once the glucose and the biomass concentrations into the reactor have been estimated using the Luenberger observer (18), we are able to implement the Super-Twisting observer (10) to estimate the glucose concentration at the reactor input. 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.

Figure 6 shows the 'real' glucose concentration at the reactor input (in solid blue) and the estimated one (in dashed black). As can be observed, the glucose concentration remains close to the 'real' one along the simulation, however, after the day 17 even if the estimated glucose follows the 'real' one, the estimation is not correct at all. This may be caused by the lack of an exact estimation of both the glucose and the

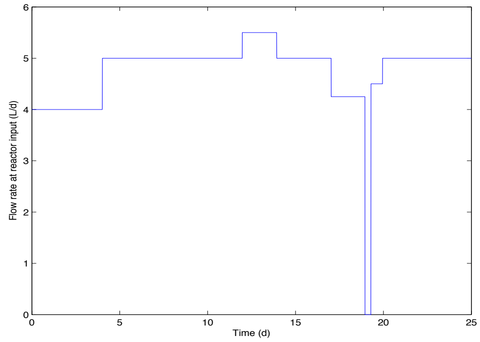

Fig. 5: Flow rate at the reactor input.

biomass inside the reactor, specially of the biomass between days 17 and 20 as shown in figure 4.

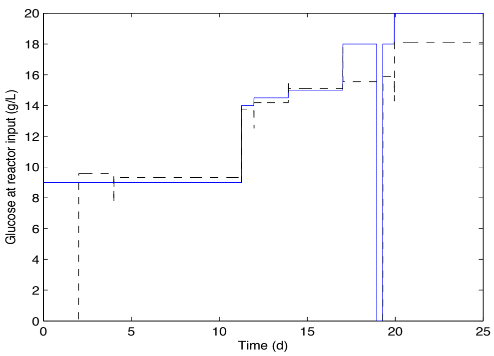

Fig. 6: Estimation of the glucose concentration at the reactor input. In blue solid line the 'real' concentration and in black dashed line the estimated one.

Figure 7 shows the estimation error of the glucose concentration at the reactor input. As can be regarded, after the estimation has started (day 2), the estimation error remains around zero but after the day 17 the error estimation grows around $2g/L$.

VI. Conclusions and perspectives

In this work, a coupled observer to estimate the glucose concentration at the input of a hydrogen production reactor 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. However, the estimation was not correct at all in the last eight days as consequence of not exact estimations of both, glucose and biomass inside the reactor. It suggests that the Luenberger observer must be improved maybe by considering another norm, as the H_∞ one, to minimize the influence of the disturbance on the error estimation.

After simulating this estimation strategy we are ready to implement it at the laboratory in the real

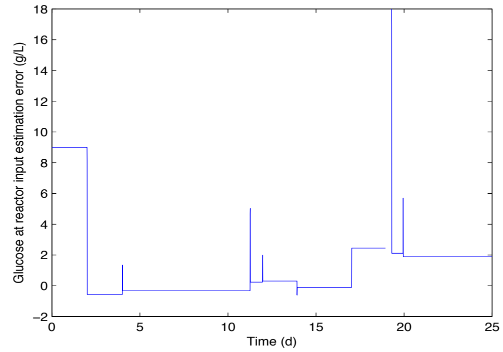

Fig. 7: Estimation error of the glucose concentration at the reactor input.

hydrogen production reactor. First, the model will have to be calibrated for the reactor. Once the observer is validated with real data, the optimization problem to maximize the hydrogen productivity will can be solved with variable glucose concentrations at the reactor input.

VII. Acknowledgments

This research was financed by CONACYT (project 100298). The first author gratefully acknowledges the support of CONACYT in the framework of a postdoctoral grant.

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