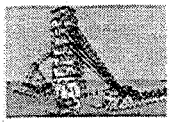

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STATE OBSERVERS FOR PROCESSES WITH UNCERTAIN KINETICS

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Abstract: This paper deals with the design of observers that are aimed at dealing with the uncertainty related to the process kinetics. Two approaches are proposed. The first approach consists of using the unknown (kinetic) parameters as extra design parameters in order to guarantee zero steady-state observation error of the estimated process variables. The second approach includes the on-line estimation of the unknown (kinetic) parameters in an adaptive observer fra- mework. The stability of the adaptive observer is analyzed and the performance are illustrated in numerical simulations.
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1. INTRODUCTION

A key question in process control is how to monitor reactant and product concentrations in a reliable and cost effective manner. However, it appears that, in many practical applications, only some of the concentrations of the components involved and critical for quality control are available for on-line measurement. For instance, dissolved oxygen concentration in bioreactors, temperature in non-isothermal reactors and gaseous flowrates are available for on-line measurement while the values of the concentrations of products, reactants and/or biomass are often available via off-line analysis. An interesting alternative which circumvents and exploits the use of a model in conjunction with a limited set of measurements is the use of state observers. An important difficulty when applying state observers to (bio)chemical processes is related to the uncertainty of (some of) the terms in the models used to describe their dynamics. Simply speaking with respect to the above remark, two classes of state observers for (bio)chemical processes can be found presently in the literature. The first class of observers (including classical observers like Luenberger and Kalman observers, and nonlinear observers)(e.g. (Doyle III, 1997)) are based on a perfect knowledge of the model structure. As it will be illustrated in Section 2, uncertainty in the model parameters for instance can generate possibly large bias in the estimation of the unmeasured states. A second class of observers, called *asymptotic observers* ((Bastin and Dochain, 1990), (Dochain *et al.*, 1992)) is based on the idea that the uncertainty in (bio)process models lies in the process kinetics models. The design of these observers is based on the mass and energy balances without the knowledge of the process kinetics being necessary. This class of observers has resulted in a wide variety of applications in chemical and biochemical processes. The potential drawback of the asymptotic observers is the rate of convergence of the estimation which fully depends on the operating conditions. The objective of this paper is to introduce alternative solutions of state observation of (bio)processes in a situation which is intermediate to those mentioned hereabove, i.e. when the kinetics model structure is known but its parameters are badly known. Two approaches are proposed. The first approach (Section 3) consists

of using the badly known kinetic parameters as extra design parameters in order to guarantee zero steady-state observation error of the estimated process variables. The second approach (Section 4) includes the on-line estimation of the badly known kinetic parameters in an adaptive observer framework. The stability of the adaptive observer is analyzed, and the performance of both observers are illustrated via numerical simulations. A generalization of both approaches is presented in Section 5.

2. PERFORMANCE OF CLASSICAL OBSERVERS IN PRESENCE OF MODEL UNCERTAINTY

Let us derive the general structure of state observers. Let us consider the following nonlinear state space model :

$$\frac{dx}{dt} = f(x,u) \tag{1}$$

The measured variables, denoted y, are related to the process dynamical model by the following relation : $y = h(x)$. The general structure of a state observer is then written as follows :

$$\frac{d\hat{x}}{dt} = f(\hat{x},u) + K(\hat{x})(y-\hat{y}) \tag{2}$$

where $\hat{x}$ and $\hat{y}$ are the on-line estimation of x and y given by the state observer : $\hat{y} = h(\hat{x})$. and where K is the "gain" of the observer. The design of the state observer consists of choosing an appropriate gain $K(\hat{x})$. The above state observer was originally developed for linear problems. Because of the nonlinear characteristics of the (bio)process dynamics, it is of interest to extend these concepts and exploit particular structures for (bio)chemical engineering application problems. The design of the gain matrix K is based on a linearized version (the linearized tangent model) of the process dynamics observation error (computed from a Taylor's series expansion of a state space model around some equilibrium point). If we define the observation error e as follows : $e = x - \hat{x}$, the dynamics of the error observation are readily derived from equations (1) and (2) :

$$\begin{aligned}\frac{de}{dt} &= f(\hat{x}+e,u) - f(\hat{x},u) \\ &\quad -K(\hat{x})(h(\hat{x}+e) - h(\hat{x}))\end{aligned} \tag{3}$$

If we consider the linearization of the above equation around the observation error $e = 0$, we obtain:

$$\frac{de}{dt} = (A(\hat{x}) - K(\hat{x})L(\hat{x}))e \tag{4}$$

where $A(\hat{x})$ and $L(\hat{x})$ are respectively equal to:

$$A(\hat{x}) = [\frac{\partial f}{\partial x}]_{x=\hat{x}},\ L(\hat{x}) = [\frac{\partial h}{\partial x}]_{x=\hat{x}} \tag{5}$$

Thus the design problem can be formulated as the choice of the matrix $K(\hat{x})$ such that the linearized error dynamics (4) has desired properties. This has resulted in two typical state observation designs : the extended Luenberger observer, and the extended Kalman observer. The word "extended" obviously emphasizes that these observers are extensions of the original linear versions to nonlinear systems.

Let us now illustrate the performance of a classical observer when some of the model parameters are badly known. Let us consider here the extended Luenberger observer applied to the estimation of the biomass concentration X from measurements of the substrate concentration S in a simple microbial growth process[1]. The model dynamics in a CSTR (continuous stirred tank reactor) are given by the following equations :

$$\frac{dS}{dt} = -k_1\mu X + DS_{in} - DS \tag{6}$$

$$\frac{dX}{dt} = \mu X - DX \tag{7}$$

where k_1, μ, D, S_{in} represent the yield coefficient, the specific growth rate (h^{-1}), the dilution rate (h^{-1}), and the influent substrate concentration (g/l), respectively. Let us consider Monod kinetics $\mu = \mu_{max}S/(K_S + S)$ with μ_{max} the maximum specific growth rate (h^{-1}) and K_S the saturation constant (g/l). The observer equations are then equal to :

$$\begin{aligned}\frac{d\hat{S}}{dt} &= -k_1\tilde{\mu}_{max}\frac{\hat{S}}{\tilde{K}_S+\hat{S}}\hat{X} + DS_{in} - D\hat{S} \\ &\quad +K_1(S-\hat{S})\end{aligned} \tag{8}$$

$$\frac{d\hat{X}}{dt} = \tilde{\mu}_{max}\frac{\hat{S}}{\tilde{K}_S+\hat{S}}\hat{X} - D\hat{X} + K_2(S-\hat{S}) \tag{9}$$

$\hat{S}$ and $\hat{X}$ represent the estimations of S and X given by the observer. The parameters $\tilde{\mu}_{max}$ and $\tilde{K}_S$ used in the observer computation may be different from their "true" values μ_{max} and K_S. In the extended Luenberger observer (ELO), the gains K_1 and K_2 are selected as follows :

$$K_1 = \lambda_1 + \lambda_2 - k_1\frac{\tilde{K}_S\tilde{\mu}_{max}\hat{X}}{(K_S+\hat{S})^2} + \frac{\tilde{\mu}_{max}^2\hat{S}}{\tilde{K}_S+\hat{S}} - 2D \tag{10}$$

$$K_2 = \frac{\tilde{K}_S+\hat{S}}{k_1\tilde{\mu}_{max}\hat{S}}[-\lambda_1\lambda_2 + (\lambda_1+\lambda_2)(D - \frac{\tilde{\mu}_{max}\hat{S}}{\tilde{K}_S+\hat{S}})$$

[1] The choice of the extended Luenberger is obviously arbitrary and is not based on any priori idea about its advantages and drawbacks. The choice of the bioractor example is also arbitrary, yet it will be used throughout the paper as the illustration support.

$$-(D - \frac{\tilde{\mu}_{max}\hat{S}}{\tilde{K}_S + \hat{S}})^2 + k_1 \frac{\tilde{\mu}_{max}\tilde{K}_S\hat{S}\hat{X}}{(\tilde{K}_S + \hat{S})^3}] \quad (11)$$

in order to have observer dynamics assigned to desired values λ_1 and λ_2. Let us test the performance of the observer with a wrong value of one kinetic parameter. The numerical simulation conditions are the following:

$$k_1 = 2,\ \mu_{max} = 0.33\,h^{-1},\ K_S = 5\,g/l,\ S_{in} = 5\,g/l$$
$$D = 0.05\,h^{-1},\ X(0) = 1\,g/l,\ S(0) = 0.5\,g/l$$

The observer has been initialized with $\hat{S}(0) = S(0)$ and $\hat{X}(0) = 0$. Figure 1 shows the estimation results with 10 % error on K_S ($\tilde{K}_S$ = 4.5 g/l instead of 5) for two sets of design parameters K_1 and K_2 (one corresponding to $\lambda_1 = \lambda_2$ = -0.1 ("slow" dynamics), the other for $\lambda_1 = \lambda_2$ = -10 ("fast" dynamics))[2]. The results are quite typical of classical observers but also of any "high gain" observers for nonlinear systems : the higher the gain, the worse the state estimation. Indeed high gain (fast dynamics) will result in a good estimation of the measured variable (here S)(it is impossible to distinguish on the figure between S and $\hat{S}$!) while rejecting the parameter uncertainty on the estimated variable (here X). This simple example shows that there is a need to develop observers that can handle parameter uncertainty, a typical situation encountered in (bio)chemical process applications.

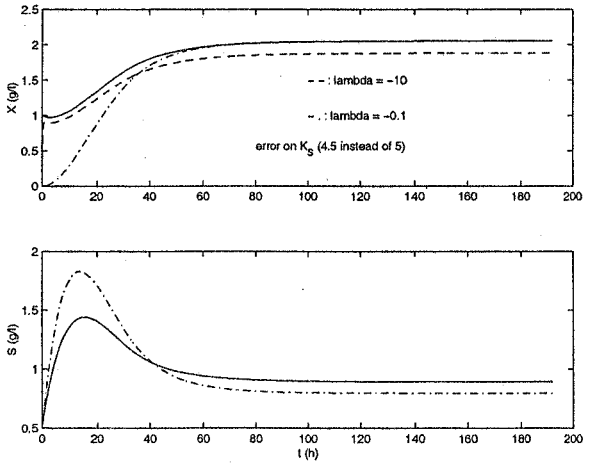

Fig. 1. *Extended Luenberger observer with a wrong value of K_S (initial transient)(- : "true" simulated values)*

3. STATE OBSERVER WITH UNKNOWN PARAMETER AS DESIGN PARAMETER

The first approach that we propose in this paper is based on the following idea : why not using the badly parameters as extra design observer parameters in order to guarantee (at least) zero steady-state observation errors for the unmeasured variables? Let us denote the badly known parameters by θ. The process dynamics (1) can be rewritten as follows :

$$\frac{dx}{dt} = f(x, u, \theta) \quad (12)$$

If we consider that the output vector consists of state variables (as it is often the case in (bio)processes), we can define a state partition with the measured variables ($y = x_1$) and the unmeasured variables, x_2 :

$$\frac{dx_1}{dt} = f_1(x, u, \theta) \quad (13)$$
$$\frac{dx_2}{dt} = f_2(x, u, \theta) \quad (14)$$

The observer design remains basically the same, but now we choose θ such that $x_2 - \hat{x}_2$ is equal to zero in steady state, i.e.:

$$\theta : (x_2(\theta) - \hat{x}_2(\theta))_{ss} = 0 \quad (15)$$

Let us illustrate this idea on the simple microbial growth example. The objective is to select one of the kinetic parameter used in the observer such that the estimation error is equal to zero in steady-state. Let us first consider that the badly known parameter is the saturation constant K_S (this means that we use $\tilde{K}_S$ and μ_{max} in the observer equations). Then the dynamics of the observation errors are equal to :

$$\frac{d}{dt}\begin{bmatrix} e_S \\ e_X \end{bmatrix} = \begin{bmatrix} -D - k_1\tilde{\alpha}X - K_1 & -k_1\tilde{\alpha}\hat{S} \\ \tilde{\alpha} - K_2 & \tilde{\alpha}\hat{S} - D \end{bmatrix}\begin{bmatrix} e_S \\ e_X \end{bmatrix} + \begin{bmatrix} -k_1 SX \\ SX \end{bmatrix} e_\alpha \quad (16)$$

with :

$$\tilde{\alpha} = \frac{\mu_{max}}{\tilde{K}_S + \hat{S}},\ e_\alpha = \mu_{max}[\frac{1}{K_S + S} - \frac{1}{\tilde{K}_S + \hat{S}}]$$

e_S and e_X are the estimation errors on S and X. As a matter of illustration, if we consider the ELO, the gains K_1 and K_2 are chosen from equations (10)(11). Let us set de_S/dt, de_X/dt to zero. Then, e_X in steady-state, $\bar{e}_X$, is given by the following expression :

$$\frac{(k_1K_2 + K_1 + D)SXe_\alpha}{(D - \tilde{\alpha}\hat{S})(D + K_1 + k_1\tilde{\alpha}X) + k_1\tilde{\alpha}\hat{S}(\tilde{\alpha}X - K_2)}$$

We note that $\bar{e}_X$ will be equal to zero if $k_1K_2 + K_1 + D = 0$. This gives the following expression for $\tilde{K}_S$:

$$\tilde{K}_S = -\hat{S} + \frac{\mu_{max}D\hat{S}}{D^2 - (\lambda_1 + \lambda_2)D + \lambda_1\lambda_2} \quad (17)$$

[2] similar results are obtained with an error on μ_{max}.

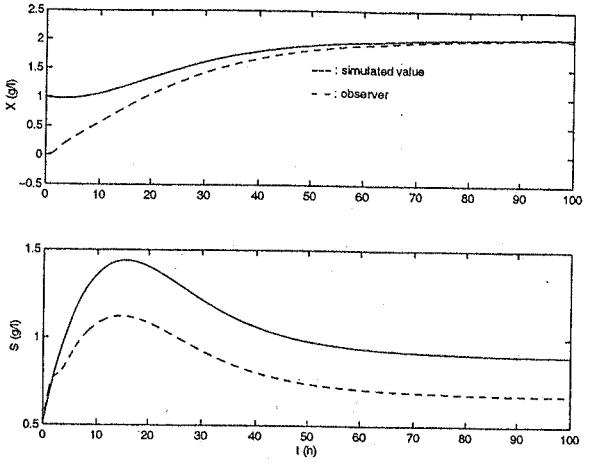

Fig. 2. *Extended Luenberger observer with K_S computed from (17)(initial transient)(- : "true" simulated values; - - : estimates)*

By using a similar approach, if μ_{max} is assumed to be badly known instead of K_S, the value of $\tilde{\mu}_{max}$ in the observer that guarantees zero steady-state error for the estimation of X is given by the following relationship :

$$\tilde{\mu}_{max} = \frac{(D^2 - (\lambda_1 + \lambda_2)D + \lambda_1\lambda_2)(K_S + \hat{S})}{D\hat{S}}$$

Figure 2 illustrates the behaviour of the ELO with $\tilde{K}_S$ given by equation (17) for $\lambda_1 = \lambda_2 =$ -0.2. It shows the convergence of the observer when $\hat{X}(0)$ = 0. The process is assumed to be initially in steady state ($X(0) = 2.054$ g/l, $S(0) = 0.893$ g/l); the observer has been initialized with the correct value for $\hat{S}$, and a wrong value for $\hat{X}$ (= 1 g/l). Note that, as expected, the estimate of X (dotted line) converges to the "true" simulated value. This is obviously done at the price of a biased estimate of the measured variable S.

Our numerical experience with different kinetic models and estimation problems tell us that the gains of the observer have to be selected not too large in order to avoid strange transient behaviour of the observer. And we have not been able so far to obtain satisfactorily (i.e. under realistic conditions) theoretical stability and convergence properties for this approach.

4. ADAPTIVE STATE OBSERVER

The second approach that we propose in order to handle (kinetic) parameter uncertainty in the state observation of (bio)chemical processes is the design of adaptive observers, i.e. observers that estimate also the badly known parameters (e.g. (Bastin and Dochain, 1990), (Chen, 1990)). One of the original feature of the present adaptive observers is to consider a nominal process model, i.e. a model with nominal values of the badly known parameters.

For simplicity we consider here that the badly parameters are such that the process models are linear in these parameters. Then we can write the right hand side of (12) as follows :

$$f(x, u, \theta) = \bar{f}(x, u, \bar{\theta}) + b(x, u)\Delta\theta \qquad (18)$$

From the above equations and the observer equations (2), the adaptive observer is readily obtained (by considering the badly known parameters (here $\Delta\theta$) as unmeasured states with dynamics equal to zero) :

$$\frac{d\hat{x}}{dt} = \bar{f}(\hat{x}, u, \bar{\theta}) + b(\hat{x}, u)\widehat{\Delta\theta} + K(y - \hat{y}) \qquad (19)$$

$$\frac{d\widehat{\Delta\theta}}{dt} = \Gamma(y - \hat{y}) \qquad (20)$$

Some important remarks are probably necessary at this point. Although the design of adaptive observers has been a very active research field in the eighties, their theoretical analysis may become easily highly complex. Moreover our experience shows that their application to processes is indeed so far quite disappointing because they are very difficult to tune properly in practice. That's why we have limited our study here to the following items :

1) to base the design on a model with nominal values of the badly known parameters;

2) to consider here only models linear in the badly known parameters;

3) to allow only one badly known parameter per measured variable;

4) to consider the averaging (see e.g. (Mareels and Polderman, 1996)) as a key tuning rule for the adaptive observer.

Item 1 is important to increase the flexibility on the observer dynamics. Item 2 is only an a priori choice that simplifies the approach. Item 3 is probably the most essential assumption in order to have some guarantee of successful implementation of the observer, and is rather easy to understand from a practical viewpoint : how can one expect to handle properly uncertainty on different kinetics and distinguish between them if there is not a sufficient amount of information about them, in particular one indepedent information per independent unknown. Finally, item 4 is also a key issue in the implementation of the adaptive observer : one important underlying idea of averaging is that the dynamics of the parameter adaptation have to be slower than the dynamics of the rest of the observer.

In the rest of the section we shall consider the same example as before (simple microbial growth) on which we shall perform the theoretical analysis of the adaptive observer and illustrate its performance in numerical simulation. Assume that μ_{max} is the badly known parameter, with : $\mu_{max} = \bar{\mu}_{max} + \Delta\mu_{max}$, where $\bar{\mu}_{max}$ is a nominal value of μ_{max}. Then equation (18) specializes as follows:

$$\frac{dS}{dt} = -k_1\bar{\mu}_{max}\frac{SX}{K_S+S} + DS_{in} - DS - \frac{k_1 SX}{K_S+S}\Delta\mu_{max}$$

$$\frac{dX}{dt} = \bar{\mu}_{max}\frac{SX}{K_S+S} - DX + \frac{SX}{K_S+S}\Delta\mu_{max}$$

At this point we consider an asymptotic observer for estimating the value of X that appears in the regressor (i.e. the mulplicative term) of $\Delta\mu_{max}$. Its introduction is fully motivated by the theoretical analysis that will be performed herebelow. The design of asymptotic observers has been first introduced for bioprocesses (e.g. (Bastin and Dochain, 1990)), then extended to (nonisothermal) chemical reactors (Dochain *et al.*, 1992). The asymptotic observer is based on a state transformation that specializes here as follows : $Z = S + k_1 X$. Its dynamical equation is readily derived from the model equations (6),(7) :

$$\frac{dZ}{dt} = -DZ + DS_{in} \tag{21}$$

The important feature of the above equation is its independence with respect to the process kinetics. We use the above equation to compute Z, and then inverse the equation of Z to obtain an estimate of X :

$$X_e = \frac{Z-S}{k_1} \tag{22}$$

Equations (21)(22) are here the asymptotic observer. The adaptive observer is then equal to :

$$\frac{d\hat{S}}{dt} = -k_1\bar{\mu}_{max}\frac{S\hat{X}}{K_S+S} + DS_{in} - DS - \frac{k_1 SX_e}{K_S+S}\widehat{\Delta\mu_{max}} + K_1(S-\hat{S}) \tag{23}$$

$$\frac{d\hat{X}}{dt} = \bar{\mu}_{max}\frac{S\hat{X}}{K_S+S} - D\hat{X} + \frac{SX_e}{K_S+S}\widehat{\Delta\mu_{max}} - K_2(S-\hat{S}) \tag{24}$$

$$\frac{d\widehat{\Delta\mu_{max}}}{dt} = -\gamma(S-\hat{S}) \tag{25}$$

The analysis of the theoretical stability and convergence properties are based on the estimation error dynamics. If we define :

$$e_S = S - \hat{S},\ e_X = X - \hat{X} \tag{26}$$

$$e_\mu = \Delta\mu_{max} - \widehat{\Delta\mu_{max}} \tag{27}$$

these are written as follows :

$$\frac{de}{dt} = Ae + Be_{Xe} \tag{28}$$

with :

$$A = \begin{bmatrix} -K_1 & -k_1\frac{\bar{\mu}_{max}S}{K_S+S} & -k_1\frac{SX_e}{K_S+S} \\ K_2 & \frac{\bar{\mu}_{max}S}{K_S+S} - D & \frac{SX_e}{K_S+S} \\ \gamma & 0 & 0 \end{bmatrix}$$

$$e = \begin{bmatrix} e_S \\ e_X \\ e_\mu \end{bmatrix},\ B = \begin{bmatrix} -k_1\frac{\Delta\mu_{max}S}{K_S+S} \\ \frac{\Delta\mu_{max}S}{K_S+S} \\ 0 \end{bmatrix},\ e_{Xe} = X - X_e$$

From the theory of the asymptotic observers, we know that e_{Xe} will tend asymptotically to zero : $\lim_{t\to\infty} e_{Xe} = 0$. We also know ((Bastin and Dochain, 1990)) that the matrix B is bounded. Similarly, if K_1, K_2 and γ are bounded, then A is bounded. Therefore the error dynamics are a time-varying system with an input going asymptotically to zero. If the state matrix A is asymptotically stable, we can use a classical stability result (e.g. (Willems, 1970), p.55) to state that the estimation errors will tend asymptotically to zero. Let us check now that A is a stable matrix. Its characteristic polynomial $\det(\lambda I - A)$ is equal to :

$$\lambda^3 + \lambda^2(K_1 + D - \frac{\bar{\mu}_{max}S}{K_S+S}) + \lambda(K_1(D - \frac{\bar{\mu}_{max}S}{K_S+S}) + K_2k_1\frac{\bar{\mu}_{max}S}{K_S+S} + \gamma k_1\frac{SX_e}{K_S+S}) + \gamma k_1 D\frac{SX_e}{K_S+S}$$

It is then routine to check that A is asymptotically stable via a proper choice of the gains K_1, K_2, and γ, e.g. if we assign the dynamics of the observer with the following three eigenvalues λ_1, λ_2, λ_3. Figure 3 illustrates the performance of the observer under the same initial and operating conditions as in Figure 2, but with a 10% error on μ_{max}. The gains have been chosen primarily to assign the dynamics with $\lambda_1 = \lambda_2 = \lambda_3 = 5$ h^{-1}, then γ has been reduced by a factor 20 to follow the averaging recommendations (the factor is somewhat arbitrary (10 would have been good too for instance), it just gives a rough idea of a typical value for γ). Note that the adaptive observer (which assumes the knowledge of the kinetics model) is able to converge faster than the asymptotic observer (which ignores the kinetics model). It is also worth noting the adaptive observer (23)(24)(25) is capable of handling nonlinear uncertainties like those on K_S, as it illustrated in Figure 4, which presents a numerical simulation performed under the same conditions as in Figure 3, but with a 10% error on K_S.

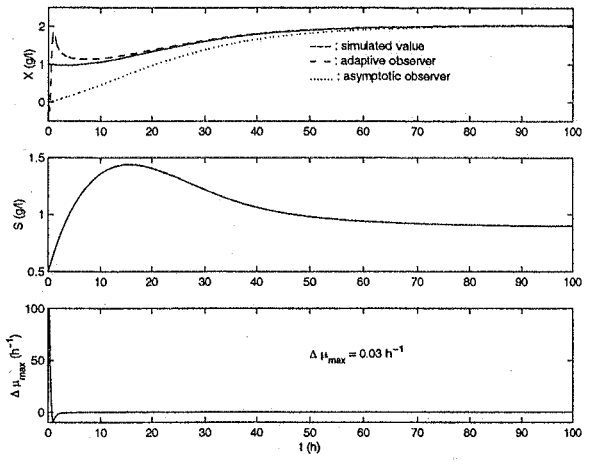

Fig. 3. *Adaptive observer (initial transient)*

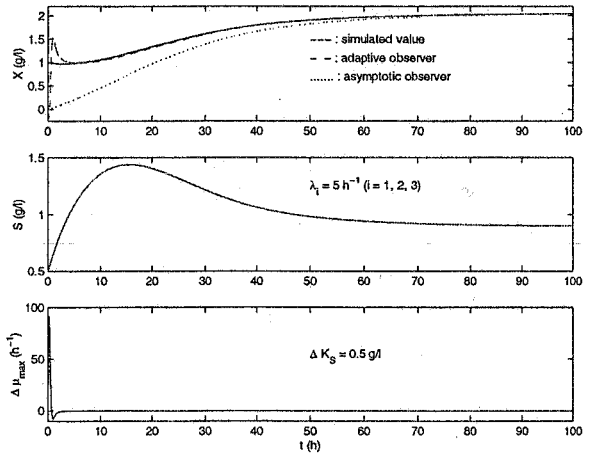

Fig. 4. *Adaptive observer (10% error on K_S)*

5. GENERALIZATION

The generalization of both proposed observers is based on the General Dynamical Model introduced in (Bastin and Dochain, 1990) (Dochain *et al.*, 1992):

$$\frac{dx}{dt} = -Dx + Kr + U \qquad (29)$$

where x, K, r and U represent the process components, the stoichiometric or yield coefficient matrix, the reaction rate vector, and the external exchange vector, respectively. U includes external feedrates, gaseous outflow rates, and thermal exchanges (for non isothermal reactors). x and K includes the temperature and the heat of each reaction ΔH. If we consider that the measured outputs y are process components (with possibly the temperature), then the part of the General Dynamical Model associated to y is written as follows :

$$\frac{dy}{dt} = -Dy + K_y r + U_y \qquad (30)$$

where K_y and U_y gather the rows of K and U related to y. The key assumptions at this point are to consider that the number of measured components is (at least) equal to the number of uncertain kinetics, and that the measured components are independent (this basically implies that the submatrix K_y is full rank). The important step in the generalization consists then of introducing the following state transformation (Perrier *et al.*, 1999):

$$\zeta = K_y^{-1} y \qquad (31)$$

This transformation decouples all the kinetics terms and associates each of them to only one variable ζ. Indeed equation (30) is rewritten as follows :

$$\frac{d\zeta}{dt} = -D\zeta + r + K_y^{-1} U_y \qquad (32)$$

It is then straightforward to extend the design of both observers introduced in sections 3 and 4 to each decoupled system (ζ_i, r_i).

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