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# State and parameter estimation in chemical and biochemical processes: a tutorial

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**Abstract**

This paper aims at giving an overview of available results of state and parameter approaches for chemical and biochemical processes. It is largely organized as a tutorial and starts with a brief reminder concerning the design of extended Luenberger (ELO) and Kalman (EKO) observers, followed by an illustrative nonlinear observer algorithm. Evaluation of the performance of classical observers in presence of model uncertainties will serve as a basis for the motivation of designing asymptotic and interval observers, that do not require the knowledge of the process kinetics. The design of state observers with known kinetic models but uncertain kinetic parameters will then be considered via suggestions of improvements of the EKO and the introduction of two other types of observers (observers where the unknown parameters are used as design parameters; adaptive observers). Finally, the design of on-line parameter estimation schemes will be introduced. One of the objectives of the present survey is also to suggest new research directions.



*Keywords:* State estimation; Parameter estimation; Chemical processes; bioprocesses; Parameter uncertainty

## 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 flow rates are available for on-line measurement while the values of the concentrations of products, reactants and/or biomass are often available via on-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.[1]

The design and application of state observers in (bio)processes has been an active area over the past decades [23]. 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 described 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. [23]) are based on perfect knowledge of the model structure. Classical observers, particularly the extended Kalman filter, have found applications in some (bio)chemical processes (e.g. [48,37,30,18,38,47,36,10]). One problem with the above observers is that the theory for the extended Luenberger and Kalman observers and for the nonlinear observers is developed using perfect knowledge of the system parameters, in particular of the process kinetics: it is difficult to develop error bounds and there is often a

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[1] In the scientific literature, the expression *software sensors* tends to be more and more largely used for state and parameter estimators since these provide *software* measurements of unmeasured variables and/or unknown parameters on the basis of the knowledge of the process dynamics (the dynamical model) and on the few available on-line measurements. This expression has been first used in a European project in the middle of the eighties [4].

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large uncertainty on these parameters. As it will be illustrated below, 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* ([3,20]) (see Section 3.1 for a motivation of the terminology) 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 but without requiring the knowledge of the process kinetics. The potential drawback of the asymptotic observers is the rate of convergence of the estimation which fully depends on the operating conditions. There is therefore room to design alternative solutions of state observation of (bio)processes in a situation which is intermediate to those mentioned here above, i.e. when the kinetics model structure is known but its parameters are poorly known.

Because of the potentially large uncertainty about the knowledge of the values of some of the process parameters, it is also important to use techniques that are able to combine state observation with parameter estimation.

In summary, one major challenge that parameter and state estimators applied to chemical and biochemical processes is to handle the model and measurement uncertainties: this will be the main object of the present tutorial. The paper is therefore organized as follows. In Section 2 the basic design concepts of state observers for extended Luenberger and Kalman and for one nonlinear observer will be introduced. In the same section we illustrate the performance limitations of these observers in presence of uncertain model parameters. Section 3 will introduce asymptotic observers and their extensions to interval observers (based on the notion of cooperative systems) as an alternative when the process kinetics are unknown. Section 4 will be dedicated to the design of observers when the kinetics model structure is known but not some of the model parameters. Section 5 will present a comparison of the eight state observers presented in Sections 2, 3 and 4. Section 6 will concentrate on the design of parameter estimators independent of the state observation. Section 7 will present a few real-life applications of some methodologies presented in the preceding sections. Section 8 will discuss already existing solutions for the state and parameter estimation in batch processes but for which another key issue is to handle properly the time limitation of the process operation) as well as future perspectives. The paper is largely written as a tutorial. One common example will be considered for all the state observers of Sections 2 and 3: a non-isothermal chemical stirred tank reactor with one reactant and one product (when needed):

$$A \rightarrow bB \tag{1}$$

where $b$ is the stiochiometric coefficient. The model dynamics of the process for the reactant concentration $C_A$, the product concentration $C_B$ and the temperature $T$ are readily derived from mass and energy balance considerations that lead to the following set of differential equations:

$$\frac{dC_A}{dt} = -k_0 C_A e^{-\frac{E}{RT}} + \frac{q}{V}(C_{in} - C_A) \tag{2}$$

$$\frac{dC_B}{dt} = bk_0 C_A e^{-\frac{E}{RT}} - \frac{q}{V} C_B \tag{3}$$

$$\frac{dT}{dt} = -\frac{\Delta H}{\rho C_p} k_0 C_A e^{-\frac{E}{RT}} + \frac{q}{V}(T_{in} - T) + \frac{hA}{\rho C_p V} \times (T_w - T) \tag{4}$$

where $k_0$, $E$, $R$, $q$, $V$, $C_{in}$, $T_{in}$, $\Delta H$, $\rho$, $C_p$, $h$, $A$, $T_w$ represent the kinetic constant ($h^{-1}$), the activation energy (kJ/kmol), the ideal gas constant (kJ/kmol/K), the influent flow rate (l/h), the volume (l), the influent reactant concentration (mole/l), the influent temperature (K), the heat of reaction (kJ/kmol), the density (g/l), the specific heat (kJ/kg/K), the overall heat transfer coefficient ($W/m^2/K$), the heat transfer area ($m^2$), the heat exchanger temperature (K), respectively. We shall consider the design of state observers applied to the estimation of the reactant concentration $C$ from measurements of the temperature $T$. The numerical simulation results presented in Sections 2, 3 and 4 have been performed by considering the conditions in Table 1.

## 2. Design of classical observers

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

$$\frac{dx}{dt} = f(x, u) \tag{5}$$

The measured variables, denoted $y$, are related to the process dynamical model by the following relation:

$$y = h(x) \tag{6}$$

Table 1
Parameter and initial conditions for the numerical simulation

| Parameter | value | Parameter | value |
|---|---|---|---|
| $k_0$ | $7.2\ 10^{10}$ $min^{-1}$ | $E$ | $8.3143\ 10^4$ kJ/(kmol K) |
| $q$ | 100 l/min | $V$ | 100 l |
| $\rho$ | $10^3$ g/l | $C_p$ | 1 cal/(g K) |
| $C_{in}$ | 1 mol/l | $T_{in} = T_w$ | 350 K |
| $hA$ | $1.0329\ 10^5$ cal/(min K) | $\Delta H$ | $-2\ 10^5$ kcal/kmol |

| Variable | Initial value | Variable | Initial value |
|---|---|---|---|
| $C_A(0)$ | 0.5 mol/l | $T(0)$ | 300 K |
| $C_B(0)$ | 0.1 mol/l | | |

The general structure of a state observer is then written as follows:

$$\frac{d\hat{x}}{dt} = f(\hat{x}, u) + K(\hat{x})(y - \hat{y}) \tag{7}$$

where $\hat{x}$ and $\hat{y}$ are the on-line estimations of $x$ and $y$ given by the state observer:

$$\hat{y} = h(\hat{x}) \tag{8}$$

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. If we define the observation error $e$ as follows:

$$e = x - \hat{x} \tag{9}$$

the dynamics of the error observation are readily derived from Eqs. (5) and (7):

$$\frac{de}{dt} = f(\hat{x} + e, u) - f(\hat{x}, u) - K(\hat{x})(h(\hat{x} + e) - h(\hat{x})) \tag{10}$$

The design problem can be formulated as the choice of the matrix $K(\hat{x})$ such that the error dynamics (10) has desired properties. This has resulted in a number of state observer designs, including two classical state observation designs (the extended Luenberger observer, and the extended Kalman observer), as well as a variety of nonlinear observers (Section 2.3).

The word "extended" obviously emphasizes the fact that these observers are extensions of the original linear versions to nonlinear systems. 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 consider the linearization of the above equation around the observation error $e = 0$, we obtain:

$$\frac{de}{dt} = (A(\hat{x}) - K(\hat{x})L(\hat{x}))e \tag{11}$$

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

$$A(\hat{x}) = \left[\frac{\partial f}{\partial x}\right]_{x=\hat{x}}, \quad L(\hat{x}) = \left[\frac{\partial h}{\partial x}\right]_{x=\hat{x}} \tag{12}$$

Let us consider the design of the state observer for the non-isothermal reactor model. In order to limit the complexity of the mathematical development, only the reactant concentration and the temperature equations (2) and (4) are considered here. The output matrix $L(\hat{x})$ and the state matrix $A(\hat{x})$ of the linearized tangent model of the process dynamics are equal to:

$$L(\hat{x}) = [0 \;\; 1], \quad A(\hat{x}) = \begin{bmatrix} -\hat{a}_1 - \dfrac{q}{V} & -\hat{a}_1\hat{a}_3 \\ \hat{a}_1 a_2 & \hat{a}_1 a_2 \hat{a}_3 - \dfrac{q}{V} - \dfrac{hA}{\rho C_p V} \end{bmatrix} \tag{13}$$

with

$$\hat{a}_1 = k_0 e^{-\frac{E}{RT}}, \quad a_2 = -\frac{\Delta H}{\rho C_p}, \quad \hat{a}_3 = \frac{E\hat{C}_A}{R\hat{T}^2} \tag{14}$$

The observer equations are equal to:

$$\frac{d\hat{C}_A}{dt} = k_0 \hat{C}_A e^{-\frac{E}{RT}} + \frac{q}{V}\left(C_{in} - \hat{C}_A\right) + K_1\left(T - \hat{T}\right) \tag{15}$$

$$\frac{d\hat{T}}{dt} = \frac{q}{V}\left(T_{in} - \hat{T}\right) - \frac{\Delta H}{\rho C_p} k_0 \hat{C}_A e^{-\frac{E}{RT}} + \frac{hA}{\rho C_p V} \times \left(T_w - \hat{T}\right) + K_2\left(T - \hat{T}\right) \tag{16}$$

$\hat{C}_A$ and $\hat{T}$ represent the estimates of $C$ and $T$ given by the observer.

### 2.1. Extended Luenberger observer

In the extended Luenberger observer (ELO), the objective is to select $K(\hat{x})$ such that the linearised error dynamics (11) are asymptotically stable. This is achieved by choosing $K(\hat{x})$ such that (see e.g. [3]):

(1) the matrix $A(\hat{x}) - K(\hat{x})L(\hat{x})$ and its time derivative are bounded:

$$\left\| A(\hat{x}) - K(\hat{x})L(\hat{x}) \right\| \leqslant C_1, \quad \forall \hat{x} \tag{17}$$
$$18 \left\| \frac{d}{dt}(A(\hat{x}) - K(\hat{x})L(\hat{x})) \right\| \leqslant C_2, \quad \forall \hat{x}$$

(2) The eigenvalues of $A(\hat{x}) - K(\hat{x})L(\hat{x})$ have strictly negative real parts:

$$\mathrm{Re}(\lambda_i[A(\hat{x}) - K(\hat{x})L(\hat{x})]) \leqslant C_3 < 0, \quad \forall \hat{x} \text{ and } i = 1 \text{ to } n \tag{19}$$

where $n$ is the order of the system (5).

*Comment*: it is worth noting at this point the close relationship between the notion of state observability, "á la Kalman" for instance (e.g. [34]), and the selection of arbitrary observer dynamics: if the linearised system is not observable, it is then not possible to assign freely the dynamics of the observation error (or in other words, to have perfect estimation after some defined time), i.e. to select arbitrary eigenvalues $\lambda_i$. Note that simple sufficient conditions can be easily deduced on the basis of the structure of the process model and of the

number of considered process components and reactions [19].

In the non-isothermal reactor example, the gains $K_1$ and $K_2$ are selected as follows:

$$K_2 = -\lambda_1 - \lambda_2 - \hat{a}_1 + \hat{a}_1 a_2 \hat{a}_3 - 2\frac{q}{V} - \frac{hA}{\rho C_p V} \tag{20}$$

$$K_1 = \frac{1}{\hat{a}_1 a_2} \times \left[\lambda_1\lambda_2 - \left(\hat{a}_1 + \frac{q}{V}\right)\left(\frac{q}{V} + \frac{hA}{\rho C_p V} + K_2\right) + \hat{a}_1 a_2 \hat{a}_3 \frac{q}{V}\right] \tag{21}$$

in order to have observer eigenvalues assigned to the desired values $\lambda_1$ and $\lambda_2$.

### 2.2. Extended Kalman observer

Although the Kalman filter has been originally introduced in a stochastic framework, it can also be interpreted as the solution of a (deterministic) optimisation problem (see e.g. [34,3,14]). Indeed the design of the extended Kalman observer (EKO) consists of finding the gain matrix $K(\hat{x})$ that minimises the mean square observation error:

$$E = \int_0^t e^T e d\tau \tag{22}$$

with the dynamical model (11) (''under the constraints of the dynamical model (11)'', in the usual notations of optimisation theory).

The gain matrix $R(\hat{x})$ can be shown to be equal to:

$$K(\hat{x}) = R(\hat{x})L^T \tag{23}$$

where the $nxn$ symmetric matrix (time-varying) $R(\hat{x})$ is solution of the following dynamical Riccati matrix equation:

$$\frac{dR}{dt} = -RL^T LR + RA^T(\hat{x}) + A(\hat{x})R, \quad R = R^T, \quad R(0) = R_0 = R_0^T \tag{24}$$

Note that it is possible to have a more general formulation (e.g. [34,14]), e.g. by introducing a weighting matrix $W$ that allows different weightings for the different terms of the output error with a view to standardise the error norm, e.g. when the different components of the output error are not of the same dimension. Then the Eqs. (23) and (24) become:

$$K(\hat{x}) = R(\hat{x})L^T W \tag{25}$$

$$\frac{dR}{dt} = -RL^T WLR + RA^T(\hat{x}) + A(\hat{x})R, \quad R = R^T, \quad R(0) = R_0 = R_0^T \tag{26}$$

The EKO equations applied to the non-isothermal reactor model are those presented above in Eqs. (15) and (16) and the gain Eqs. (23) and (24) specialize as follows:

$$R = \begin{bmatrix} r_1 & r_3 \\ r_3 & r_2 \end{bmatrix} \tag{27}$$

$$K_1 = r_3 \tag{28}$$

$$K_2 = r_2 \tag{29}$$

$$\frac{dr_1}{dt} = -r_3^2 - 2\left(\hat{a}_1 + \frac{q}{V}\right)r_1 - 2\hat{a}_1\hat{a}_3 r_3 \tag{30}$$

$$\frac{dr_2}{dt} = -r_2^2 - 2\left(\hat{a}_1 a_2 \hat{a}_3 - \frac{q}{V} - \frac{hA}{\rho C_p V}\right)r_2 + 2\hat{a}_1 a_2 r_3 \tag{31}$$

$$\frac{dr_3}{dt} = -r_2 r_3 + \left(\hat{a}_1 a_2 \hat{a}_3 - \frac{q}{V} - \frac{hA}{\rho C_p V}\right)r_3 - \left(\hat{a}_1 + \frac{q}{V}\right)r_3 - \hat{a}_1\hat{a}_3 r_2 + \hat{a}_1 a_2 r_1 \tag{32}$$

### 2.3. A Nonlinear Observer

The design of nonlinear observers has been a very active research area, particularly from the seventies (see e.g. [31,32,39,25,16,17]). Most of these approaches are usually gathered under the category of ''high gain'' observers since they tend to split the dynamics into a linear part and a nonlinear part and to choose the gain of the observer so that the linear part dominates the nonlinear one.

Let us illustrate this with one nonlinear observer: the adaptive high gain observer of Bullinger et al. [8,9]. It is based on the following normal form of the process dynamics:

$$\frac{dx_1}{dt} = x_2 \tag{33}$$

$$\frac{dx_{n-1}}{dt} = x_n \tag{34}$$

$$\frac{dx_n}{dt} = \phi(x, u) \tag{35}$$

$$y = x_1 \tag{36}$$

where $\phi(x, u)$ contains the process nonlinearities. Such a normal form exists for systems of relative degree $n$ that are locally observable (see e.g. [29] for further details). The observer equations are then written as follows:

$$\frac{d\hat{x}_1}{dt} = \hat{x}_2 + p_1 k(y - \hat{y}) \tag{37}$$

$$\frac{dx_{n-1}}{dt} = \hat{x}_n + p_{n-1}k^{n-1}(y - \hat{y}) \tag{38}$$

$$\frac{d\hat{x}_n}{dt} = p_n k^n (y - \hat{y}) \tag{39}$$

$$\hat{y} = \hat{x}_1 \tag{40}$$

The gain $k$ is selected as the solution of the following differential equation (adaptive observer):

$$\frac{dk}{dt} = \gamma d^2_{c_1,c_2}(e_1(t)), \quad e_1 = y - \hat{y} \tag{41}$$

with

$$d_{c_1,c_2} = \begin{cases} c_2 - c_1 & \text{for } |y - \hat{y}| \geqslant c_2 \\ |y - \hat{y}| - c_1 & \text{for } c_1 \leqslant |y - \hat{y}| \leqslant c_2 \\ 0 & |y - \hat{y}| \leqslant c_1 \end{cases} \tag{42}$$

where $c_1 > c_2 > 0,)$, $\gamma > 0$ are design parameters. With this adaptation law, $k(t)$ is increasing as long as $|e_1(t)|$ is larger than $c_1$ and stops increasing once $|e_1(t)|$ becomes smaller than $c_1$. The adaptive observer is shown to give an observation error asymptotically bounded as follows:

$$\lim_{t\to\infty} \sup |x_i - \hat{x}_i| \leqslant \frac{2\alpha\|Q\|}{k^{n+1-i}(0)}, \quad i = 1, \ldots, n \tag{43}$$

where $\alpha$ is the upper bound of the norm of the nonlinearity $\phi(x,u)\big(\|\phi(x,u)\| \leqslant \alpha\big)$ and $Q$ is the symmetric positive denite matrix solution of the Lyapunov equation $\tilde{A}^T Q + Q\tilde{A} = -I$ with $\tilde{A}$ the state matrix of the observer error dynamics:

$$\tilde{A} = \begin{bmatrix} 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 1 \\ 0 & \cdots & \cdots & 0 \end{bmatrix} - KL \tag{44}$$

$$K = [K_1 K_2 \cdots K_n]^T \tag{45}$$

$$L = [1 \;\; 0 \cdots 0] \tag{46}$$

with $K_i = p_i k^i$ ($i = 1$ to $n$), and for which the parameters $p_i$ have been chosen so as to have a stable matrix.

In the non-isothermal reactor example, $\phi$ is equal to:

$$\begin{aligned} \phi &= \frac{d^2 T}{dt^2} \\ &= -\frac{\Delta H}{\rho C_p} k_0 e^{-\frac{E}{RT}} \left( -k_0 C_e^{-\frac{E}{RT}} + \frac{q}{V}(C_{in} - C) \right) \\ &- \left( \frac{\Delta H}{\rho C_p} k_0 \frac{EC}{RT^2} e^{-\frac{E}{RT}} + \frac{q}{V} T + \frac{hA}{\rho C_p V} T \right) \\ &\left( -\frac{\Delta H}{\rho C_p} k_0 C e^{-\frac{E}{RT}} + \frac{q}{V}(T_{in} - T) + \frac{hA}{\rho C_p V}(T_w - T) \right) \end{aligned} \tag{47}$$

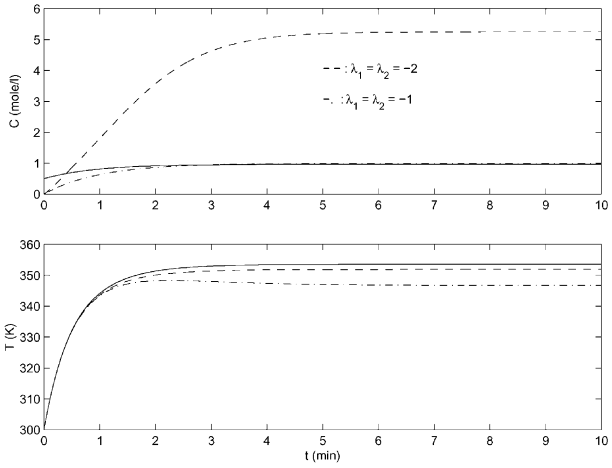


Fig. 1. Extended Luenberger observer with a wrong value of $k_0$ ("true" simulated values).

### 2.4. Performance of classical observers in presence of parameter uncertainty

Let us now illustrate the performance of a classical observer (15) and (16) when some of the model parameters are poorly known. The parameters $\tilde{k}_0$ and $\tilde{E}$ used in the observer computation may be different from their "true" values $k_0$ and $E$. Let us compute the gains with the ELO design by using Eqs. (20) and (21) where now $\hat{a}_1$ and $\hat{a}_3$ are equal to:

$$\hat{a}_1 = \tilde{k}_0 e^{-\frac{\tilde{E}}{R\hat{T}}}, \quad \hat{a}_3 = \frac{\tilde{E}\hat{C}_A}{R\hat{T}^2} \tag{48}$$

Let us test the performance of the observer with a wrong value of one of the kinetic parameter. The observer has been initialized with $\hat{C}_A(0) = 0$ mol/l and $\hat{T}(0) = T(0)$. Fig. 1 shows the estimation results with 10% error on $E$ ($\tilde{E} = 9.1457\ 10^4$ kJ/kmol/K) for two sets of design parameters $K_1$ and $K_2$ [one corresponding to $\lambda_1 = \lambda_2 = -1$ ("slow" dynamics), the other for $\lambda_1 = \lambda_2 = -2$ ("fast" dynamics)].[2] The results are quite typical of classical observers but also of any "high gain" observers for nonlinear systems: the highest the gain, the worst the state estimation. Indeed high gain (fast dynamics) will result in a good estimation of the measured variable (here $T$) while rejecting the parameter uncertainty on the estimated variable (here $C_A$). 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.

[2] Similar results are obtained with an error on $k_0$. And similar results will be provided by the EKO or with the nonlinear observer.

## 3. Asymptotic observers and interval observers

### 3.1. Asymptotic observers

The underlying idea of the asymptotic observers [3,20] is to take advantage of the structure of the dynamical models of (bio)chemical processes to rewrite part of the model in a form independent of the process kinetics. This structural property of mass and energy balance is closely related to the notion of reaction invariants [26]. The asymptotic observers belongs indeed to the class of observers for systems with unknown inputs [24,35,12,13], the unknown input being here the process kinetics.

Let us start with a general formulation of a dynamical model, obtained from mass and energy balances, for reaction systems in stirred tank reactors:

$$\frac{dx}{dt} = Yr(x) + F - Q - \frac{q}{V}x + U(T) \tag{49}$$

where $x$ holds for the vector of the concentrations of the process components [reactants, products, biomass (in bioprocesses)] and of the temperature [(for non isothermal reactors)($\dim(x) = n$)]. Then the $nxM$ matrix $Y$ is the stoichiometric coefficient matrix, $r(x)$ is the reaction rate vector [$\dim(r(x)) = M$], $F$ is the feedrate vector, $Q$ is the gaseous outflow rate vector, and $U(T)$ is the heat exchange term related to the cooling or heating system in non isothermal reactors (which is usually dependent on the temperature in the tank)[$\dim(F) = \dim(Q) = \dim(U(T)) = n$]. The most remarkable feature of the above model formulation (as every chemical engineer knows) is that the dynamics of the process is simply the sum of the process kinetics $Yr(x)$ and of the "transport" dynamics $F - Q - qx/V + U(T)$. The asymptotic observer exploits this property.

Let us consider that there are $M$ (independent[3]) reactions, and that there is $M$ measured components (possibly including the temperature $T$). Let us deffine the following state partition:

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \tag{50}$$

where $x_1$ and $x_2$ hold for the measured and unmeasured components, respectively. The above dynamical model (49) can then be rewritten as follows:

$$\frac{dx_1}{dt} = Y_1 r(x) + F_1 - Q_1 - \frac{q}{V}x_1 + U_1(T) \tag{51}$$

$$\frac{dx_2}{dt} = Y_2 r(x) + Fe - Q_2 - \frac{q}{V}x^2 + U_2(T) \tag{52}$$

If the matrix $K_1$ is full rank (which holds true if the reactions are independent and the $M$ measured components are independent), then we can define the following state transformation (closely related to the notion of reaction invariants [26]):

$$z = x_2 - Y_2 Y_1^{-1} x_1 \tag{53}$$

The dynamics of $z$ are readily derived from (51) and (52):

$$\frac{dz}{dt} = -\frac{q}{V}z + F_2 - Q_2 + U_2 - Y_2 Y_1^{-1}(F_1 - Q_1 + U_1) \tag{54}$$

This equation is independent of the reaction kinetics. This key property is very useful to design the asymptotic observer on the basis of Eqs. (53) and (54):

$$\frac{d\hat{z}}{dt} = -\frac{q}{V}\hat{z} + F_2 - Q_2 + U_2 - Y_2 Y_1^{-1}(F_1 - Q_1 + U_1) \tag{55}$$

$$\hat{x}_2 = \hat{z} + Y_2 Y_1^{-1} x_1 \tag{56}$$

The above observer requires the knowledge of the stoichiometric coefficients $Y$ (or at least the nonlinear combination of these parameters in $Y_2 Y_1^{-1}$), the feedrates $F$, the gaseous outflow rate $Q$ and the heat transfer $U$. But nothing needs to be known about the reaction kinetics. It is routine to show that the asymptotic observer is stable and convergent if $q$ is positive, or more precisely if:

$$\text{there exists } \beta > 0, \delta > 0 \text{ such that } \int_t^{t+\delta} \frac{q(\tau)}{V} d\tau > \beta \text{ for all } t \geqslant 0 \tag{57}$$

which simply means that $q$ must not remain equal to zero for too long [3,20]. A more general design is presented in Ref. [3]. The terminology *asymptotic observer* may appear somewhat confusing in regard of the traditional terminology in system theory; it has been first used in Ref. [3] to emphasize that, although the observer does not contain any estimation error driving term ("feedback") (as in the classical formulation of state observers (7)), its asymptotic stability is guaranteed even if the dynamical model is unstable (as it can happen with the exothermic chemical reactor example). As a matter of illustration, let us consider the simple example of the non isothermal reactor with the product B [Eqs. (2), (3) and (4)]. This example which is a little more complex than the one considered before allows to design the asymptotic

[3] Reversible reactions can be treated in the design of asymptotic observers as one single reaction. Similarly the number of reactions can be possibly larger than $M$, yet $M$ would correspond to the reactions for which the kinetics are assumed to be unknown or at least poorly known; the reactions with known kinetics can then have the same status in the observer design as the the other known terms, typically $F$, $Q$ and $U(T)$ (see e.g. [42] for such an approach in the context of parameter estimation).

observer with a not too much trivial example. The state transformation (53) specializes here as follows:

$$z_1 = C_A - \frac{\rho C_p}{\Delta H} T \tag{58}$$

$$z_2 = C_B + b\frac{\rho C_p}{\Delta H} T \tag{59}$$

The dynamical equations of $z_1$ and $z_2$ are readily derived from the model Eqs. (2)–(4):

$$\frac{dz_1}{dt} = -\frac{q}{V} z_1 + \frac{q}{V}\left(C_{in} - \frac{\rho C_p}{\Delta H} T_{in}\right) - \frac{hA}{\Delta H V}(T_w - T) \tag{60}$$

$$\frac{dz_2}{dt} = -\frac{q}{V} z_2 + b\frac{q}{V}\frac{\rho C_p}{\Delta H} T_{in} + b\frac{hA}{\Delta H V}(T_w - T) \tag{61}$$

In the asymptotic observer, we use the above equations to compute $z_1$ and $z_2$, and then invert the equation of $z$ to obtain an estimate of $C_A$ and of $C_B$:

$$\frac{d\hat{z}_1}{dt} = -\frac{q}{V}\hat{z}_1 + \frac{q}{V}\left(C_{in} - \frac{\rho C_p}{\Delta H} T_{in}\right) - \frac{hA}{\Delta H V}(T_w - T) \tag{62}$$

$$\frac{d\hat{z}_2}{dt} = -\frac{q}{V}\hat{z}_2 + b\frac{q}{V}\frac{\rho C_p}{\Delta H} T_{in} + b\frac{hA}{\Delta H V}(T_w - T) \tag{63}$$

$$C_{Ae} = \hat{z}_1 + \frac{\rho C_p}{\Delta H} T \tag{64}$$

$$C_{Be} = \hat{z}_2 + b\frac{\rho C_p}{\Delta H} T \tag{65}$$

Eqs. (62)–(65) are here the asymptotic observer. Here we denote by $C_{Ae}$ and $C_{Be}$ the estimates of $C_A$ and $C_B$ provided by the asymptotic observer, in order to avoid the confusion with the notation used for the state observation provided by the adaptive state observer in Section 4.4. Numerical simulation results of the state observation of $C_A$ together with those of the above asymptotic observer are given in Figs. 4 and 5 (Sections 4.4 and 5).

The asymptotic observer has resulted in a wide variety of applications in chemical and biochemical processes. Its main advantage is its full independence from the knowledge about the process kinetics. Its potential drawback is the rate of convergence of the estimation which fully depends on the operating conditions ($q(t)$).

### 3.2. Interval observers

The objective of interval observers is to generate state estimates with estimation bounds that are related to the uncertainty of the model or of the measurements [28]. The design is based on the notion of cooperative systems (see e.g. [46]). In simple words, cooperative systems are dynamical systems for which the non-diagonal terms of the Jacobian matrix are non-negative, i.e. for the dynamical system (5):

$$\frac{\partial f_i}{\partial x_j}(x) \geqslant 0, \quad \text{for } i \neq j \text{ and } t \geqslant 0 \tag{66}$$

Let us illustrate the design of interval observers in the simple non-isothermal reactor for a process where the kinetics is unknown and the influent concentration $C_{in}$ and temperature $T_{in}$ can vary between two bounds: $C_{\min} \leqslant C_{in} \leqslant C_{\max}$, $T_{\min} \leqslant T_{in} \leqslant T_{\max}$ (The bounds are assumed to be known but the vari- ations between these are not). In that case, the design of the interval observer can start from the asymptotic observer [Eqs. (55) and (56)]. It is easy to see that the dynamical system described by Eq. (55) is cooperative. Let us denote $-Y_2 Y_1^{-1}$ by $T_a$. In the interval observer with bounded feedrates $F$ [$F_{\min} \leqslant F(t) \leqslant F_{\max}$], an upper bound $z^+$ and a lower bound $z^-$ are computed:

$$\begin{aligned}\frac{dz^+}{dt} = &-\frac{q}{V}\hat{z}^+ F_{2,\max} + Q_2 + U_2 + \frac{|T_a| + T_a}{2} F_{1,\max} \\ &- \frac{|T_a| - T_a}{2} F_{1,\min} + Y_2 Y_1^{-1}(Q_1 - U_1),\end{aligned} \tag{67}$$

$$\hat{z}^+(0) = \hat{x}_2^+(0) - Y_2 Y_1^{-1} x_1$$

$$\hat{x}_2^+ = \hat{z}^+ + Y_2 Y_1^{-1} x_1 \tag{68}$$

$$\begin{aligned}\frac{dz^-}{dt} = &-\frac{q}{V}\hat{z}^- + F_{2,\min} - Q_2 + U_2 \\ &- \frac{|T_a| - T_a}{2} F_{1,\max} + \frac{|T_a| + T_a}{2} F_{1,\min} \\ &+ Y_2 Y_1^{-1}(Q_1 - U_1),\end{aligned} \tag{69}$$

$$\hat{z}^-(0) = \hat{x}_2^-(0) - Y_2 Y_1^{-1} x_1$$

$$\hat{x}_2^- = \hat{z}^- + Y_2 Y_1^{-1} x_1 \tag{70}$$

where $|T_a|$ represents the absolute values of the entries of $T_a$. The terms with the absolute value of $T_a$ are necessary to provide the correct bounds of $F_1$ (which depend on the sign of the related coefficient of the vector $T_a$) for the computation of the upper and lower bounds of $z$, as it can be noted in Table 2 here below. In other words, by doing so, we guarantee the maximum (resp. minimum) increase and the minimum (resp. maximum) decrease due to $F_1$ for $z^+$(resp. $z^-$).

In our example, in case of an exothermic reaction, these terms are equal to:

$$\begin{aligned}&\frac{|T_a| + T_a}{2} F_{1,\max} - \frac{|T_a| - T_a}{2} F_{1,\min} \\ &= \begin{bmatrix} -\dfrac{\rho C_p}{\Delta H} T_{\max} \\ b\dfrac{\rho C_p}{\Delta H} T_{\min} \end{bmatrix}\end{aligned} \tag{71}$$

Table 2
Values of the vector $T_a$ in the interval observer

| | $T_a>0$ | $T_a<0$ |
|---|---|---|
| $\frac{\lvert T_a\rvert+T_a}{2}F_{1,\max}-\frac{\lvert T_a\rvert-T_a}{2}F_{1,\min}$ | $T_aF_{1,\max}$ | $T_aF_{1,\min}$ |
| $-\frac{\lvert T_a\rvert-T_a}{2}F_{1,\max}+\frac{\lvert T_a\rvert+T_a}{2}F_{1,\min}$ | $T_aF_{1,\min}$ | $T_aF_{1,\max}$ |

$$-\frac{|T_a|-T_a}{2}F_{1,\max}+\frac{|T_a|+T_a}{2}F_{1,\min}=\begin{bmatrix}-\frac{\rho C_p}{\Delta H}T_{\min}\\ b\frac{\rho C_p}{\Delta H}T_{\max}\end{bmatrix} \tag{72}$$

Fig. 2 illustrates the behaviour in numerical simulation of the interval observers applied to the above non-isothermal reactor for the estimation of the reactant concentration $C_A$ and of the product concentration $C_B$. The interval observer has been initialized as follows:

$$C_A^+(0)=0.6\ \text{mol/l},\quad C_A^-(0)=0\ \text{mol/l}$$
$$C_B^+(0)=0.09\ \text{mol/l},\quad C_B^-(0)=0.2\ \text{mol/l}$$
$$z_1^+(0)=C_A^+(0)-\frac{\rho C_p}{\Delta H}T(0),\quad z_1^-(0)=C_A^-(0)-\frac{\rho C_p}{\Delta H}T(0)$$
$$z_2^+(0)=C_B^+(0)+b\frac{\rho C_p}{\Delta H}T(0),\quad z_2^-(0)=C_B^-(0)+b\frac{\rho C_p}{\Delta H}T(0)$$

The following bounds have been considered:

$$0.9\ \text{mol/l}\leqslant C_{in}\leqslant 1.1\ \text{mol/l},\quad 345\ \text{K}\leqslant T_{in}\leqslant 355\ \text{K} \tag{73}$$

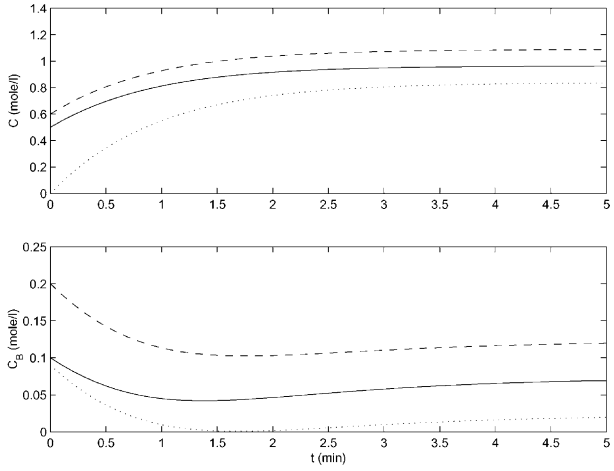


Fig. 2. Interval observer in presence of bounded in°uent reactant concentration $C_{in}$ and temperature $T_m$ (-: "true" simulated value, - -: upper bound, ...: lower bound).

We note that the interval observer provides, for the estimates of both components, bounds that are directly connected to the bounds on the process inputs. Steady-state bounds can be computed for instance from the equations in $z^+$ (67) and $z^-$ (69). If we consider for instance the bounds on the estimation of the reactant $C$, we can use Eqs. (62) and (64):

$$\left(\bar{z}_1^+\right)=C_{in}-\frac{\rho C_p}{\Delta H}T_{\max}-\frac{hA}{\Delta HV}\left(T_w-\bar{T}\right) \tag{74}$$
$$\left(\bar{z}_1^-\right)=C_{in}-\frac{\rho C_p}{\Delta H}T_{\min}-\frac{hA}{\Delta HV}\left(T_w-\bar{T}\right) \tag{75}$$

where the superscript "−" holds for steady-state values. We directly obtain the bounds for the estimation of $C_A$ from (64):

$$\left(\bar{C}_A^+\right)=\left(\bar{z}_1^+\right)+\frac{\rho C_p}{\Delta H}\bar{T} \tag{76}$$

$$\left(\bar{C}_A^-\right)=\left(\bar{z}_1^-\right)+\frac{\rho C_p}{\Delta H}\bar{T} \tag{77}$$

Interval observers have been found to be particularly useful in applications like wastewater treatment where the influent concentrations of pollutants are usually poorly known.

## 4. Observers for processes with known kinetic models and poorly known kinetic parameters

As it has been suggested so far, a frequently encountered situation in process control is when both states and parameters are unknown (or poorly known). It is then necessary to use techniques that allow to provide estimates of both. We shall start with the most classical approach: the extended Kalman observer. Since it has shown limitations in its applications, suggestions to improve its performance will be introduced. Then we shall concentrate on the design of observers when the kinetics model structure is known but not some of the model parameters, i.e. the intermediate situation between observers that require full model knowledge (Section 2) and observers that do not require any knowledge about the process kinetics (Section 3). Two approaches are introduced. The first approach consists of using the poorly known kinetic parameters as extra design parameter in order to guarantee steady-state observation error of the estimated process variables. The second approach includes the on-line estimation of the poorly known kinetic parameter in an adaptive observer framework.

### 4.1. The extended Kalman observer

The usual way to consider the problem is to extend the Kalman observer to the estimation of the unknown

parameters. The underlying idea is simple: it consists of considering the parameters as extra states with no dynamics, i.e., if we adopt the model form (5) and include the (unknown) parameters, denoted $\theta$:

$$\frac{dx}{dt} = f(x, u, \theta) \tag{78}$$

In the present context, this means that we have an augmented state $\tilde{x} = [x\ \theta]^T$ whose dynamics is given by:

$$\frac{d\tilde{x}}{dt} = \tilde{f}(\tilde{x}, u) \tag{79}$$

with:

$$\tilde{f}(\tilde{x}, u) = \begin{bmatrix} f(x, u, \theta) \\ 0 \end{bmatrix} \tag{80}$$

Then the design of the EKO follows the same line of reasoning as the one presented in Section 2.2.
Agrawal and Bonvin [2] suggest various recommendations and modifications in order to improve the performance of the extended Kalman filter, e.g.

As been pointed out in [1], the inherent linearization of extended Kalman observer design can limit its applicability to (bio)chemical processes e.g. when the states undergo large variations or if the process are largely unknown. Bonvin and coworkers [1,15,2] have suggested several options to improve its applicability:

- choice of a small initial value of the covariance matrix to eliminate the possible inadvertant reliance on an unreliable tuning (at the risk of poor convergence);
- choice of a small value of the system noise covariance when the measurement nonlinearities lead to more severe approximation than the system nonlinearities;
- use of random-ramp models instead of random-walk models for drifting parameters;
- use of dynamic variance terms for state and parameters that change at known time instants;
- use of a dynamic collector;
- use of simplified kinetic models for higher-order chemical kinetics;
- decoupling of the parameter and state estimation, and estimation of the parameter uncertainty from prediction residuals used to modify the state error covariance.

The first two recommendations deal with the initialization of the EKO: these are particularly important for batch process applications (Section 8). The third one proposes to modify the assumption of constant (or random-walk, in a stochastic context) parameters by the assumption of a linear dynamics for drifting parameters:

$$\frac{d\theta}{dt} = a \tag{81}$$

$$\frac{da}{dt} = 0 \tag{82}$$

For parameters that change stepwise at known instants, the recommendation is to adapt the variance (i.e. the entry of $R$ corresponding to the parameter) via a first order model with a step as an input.

The last recommendation is largely discussed in Ref. [2]. It basically suggests to separate the parameter estimation from the state estimation, and to perform an estimation of the parameter uncertainty from the prediction residuals for the model used by the parameter estimator and to include in the state estimator to modify the state error covariance.

### 4.2. State observer with the unknown parameters as design parameters

The approach proposed in Ref. [21,22] is based on the following idea: use the poorly known parameters as extra design observer parameters in order to guarantee (at least) zero steady-state observation errors for the unmeasured variables?

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, $x_2$, then Eq. (78) becomes:

$$\frac{dx_1}{dt} = f_1(x, u, \theta) \tag{83}$$

$$\frac{dx_2}{dt} = f_2(x, u, \theta) \tag{84}$$

The observer design basically follows the usual line of reasoning (Section 2), but now we choose $\theta$ such that $e_{x_2} = x_2 - \hat{x}_2$ is equal to zero at steady state, i.e.:

$$\theta : \bar{e}_{x_2} = 0 \tag{85}$$

Let us illustrate this idea with the non-isothermal reactor example. The objective is to select one of the kinetic parameter used in the observer such that the estimation error is equal to zero at steady state. Let us first consider that the poorly known parameter is the activation energy $E$ (this means that we use $\tilde{E}$ and $k_0$ in the observer equations). Then the dynamics of the observation errors are equal to:

$$\frac{de_C}{dt} = -\frac{q}{V}e_C - K_1 e_T - k_0 C_A e^{-\frac{E}{RT}} + k_0 \hat{C}_A e^{-\frac{\tilde{E}}{RT}} \tag{86}$$

$$\frac{de_T}{dt} = -\left(\frac{q}{V} + \frac{hA}{\rho C_p V} + K_2\right)e_T - \frac{\Delta H}{\rho C_p} k_0 \hat{C}_A e^{-\frac{\tilde{E}}{RT}} \tag{87}$$

$e_C$ and $e_T$ are the estimation errors on $C_A$ and $T$. As a matter of illustration, if we consider the ELO, the gains

$K_1$ and $K_2$ are chosen from Eqs. (20) and (21). Let us set $de_C/dt$ and $de_T/dt$ to zero. After elimination of $\bar{e}_T$ ($e_T$ at steady-state) in the steady-state equation of $e_C$, then $\bar{e}_C$ ($e_C$ at steady-state) is given by the following expression:

$$\bar{e}_C = -\frac{K_2 - \frac{\Delta H}{\rho C_p}K_1 + \frac{q}{V} + \frac{hA}{\rho C_p V}}{\frac{q}{V}\left(K_2 + \frac{q}{V} + \frac{hA}{\rho C_p V}\right)} \times \left(k_0 C_A e^{-\frac{E}{RT}} - k_0 \hat{C}_A e^{-\frac{\tilde{E}}{R\hat{T}}}\right) \quad (88)$$

We note that $\bar{e}_C$ will be equal to zero if $K_2 - \frac{\Delta H}{\rho C_p}K_1 + \frac{q}{V} + \frac{hA}{\rho C_p V} = 0$. This gives the following expression for $\tilde{E}$:

$$\tilde{E} = -R\hat{T}\ln\left(\frac{-\lambda_1\lambda_2 + (\lambda_1+\lambda_2)\frac{q}{V} - \frac{q^2}{V^2}}{\frac{gk_0}{V}}\right) \quad (89)$$

By using a similar approach, if $k_0$ is assumed to be poorly known instead of $E$, the value of $\tilde{k}_0$ in the observer that guarantees zero steady-state error for the estimation of $C$ is given by the following relationship:

$$\tilde{k}_0 = \left(\frac{-\lambda_1\lambda_2 + (\lambda_1+\lambda_2)\frac{q}{V} - \frac{q^2}{V^2}}{\frac{q}{V}}\right)e^{\frac{E}{RT}} \quad (90)$$

Fig. 3 illustrates the behaviour of the ELO with $\tilde{E}$ given by Eq. (89) for $\lambda_1 = \lambda_2 = -2$. It shows the convergence of the observer when $\hat{C}(0) = 0$ mol/l. The observer has been initialized with the correct value for $\hat{T}$. Note that, as expected, the estimate of $C$ (dotted line) converges to the "true" simulated value. The figure also shows that this is obviously done at the "price" of a wrong estimate of the measured variable $T$.

### 4.3. Adaptive state observer

The last approach [21] proposed in order to handle the state observation of processes with known kinetic models and poorly known parameters is the design of adaptive observers, i.e. observers that estimate also the poorly known parameters (e.g. [3,11]). As in the extended Kalman observer (Section 4.1), the poorly known (or unknown) parameters are considered as extra states with no dynamics. One of the original feature of the present adaptive observer in comparison to those typically available in the literature is to consider a nominal process model, i.e. a model with nominal values of the poorly known parameters.

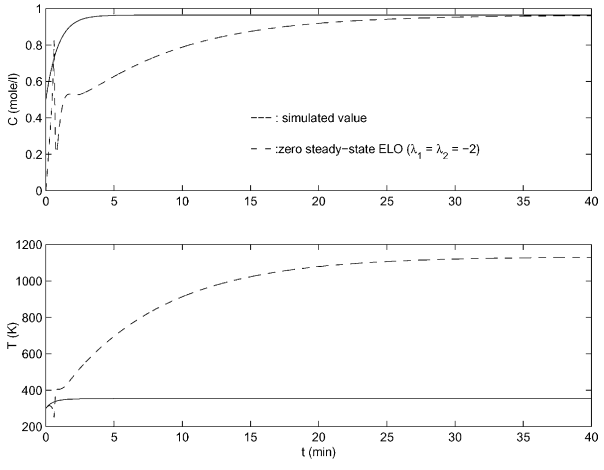


Fig. 3. Extended Luenberger observer with $\tilde{E}$ computed from Eq. (89) (initial transient) (-: "true" simulated values; - -: estimates).

For simplicity we consider here that the poorly known parameters are such that the process models are affine in these parameters. Then we can write the right hand side of (78) as follows:

$$f(x,u,\theta) = f\left(x,u,\bar{\theta}\right) + b(x,u)\Delta\theta \quad (91)$$

with $\theta = \bar{\theta} + \Delta\theta$, where $\bar{\theta}$ is the nominal value of $\theta$, and $\Delta\theta$ its deviation from the nominal value. From the above equations and the observer equations (7), the adaptive observer is readily obtained (by considering the poorly known parameters (here$\Delta\theta$) as unmeasured states with dynamics equal to zero):

$$\frac{d\hat{x}}{dt} = f\left(\hat{x},u,\bar{\theta}\right) + b(\hat{x},u)\widehat{\Delta\theta} + K(y-\hat{y}) \quad (92)$$

$$\frac{d\widehat{\Delta\theta}}{dt} = \Gamma(y-\hat{y}) \quad (93)$$

Some important remarks are probably necessary at this point. Although the design of adaptive observers has been a very active research field in the seventies and in the eighties (e.g. [33,40]), their theoretical analysis may easily become highly complex. Moreover our experience shows that their application to processes is indeed so far quite disappointing due to the difficulty of tuning them 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 poorly known parameters;
(2) to consider here only models linear in the poorly known parameters;
(3) to allow only one poorly known parameter per measured variable.

Item 1 is important to increase the flexibility of the observer dynamics: without the separation of the model kinetics into a nominal part and an unknown one, the known dynamical part of the model will reduce to the hydrodynamics for which the system will only be detectable (and not observable), and assignment of the observer dynamics will then be problematic. 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 independent information per independent unknown.

Here again we shall consider the same example as before (non-isothermal reactor) on which we shall perform the theoretical analysis of the adaptive observer and illustrate its performance in numerical simulation. Assume that $k_0$ is the poorly known parameter, with: $k_0 = \bar{k}_0 + \Delta k_0$, where $\bar{k}_0$ is a nominal value of $k_0$. Then Eqs. (2) and (4) specialize as follows:

$$\frac{dC_A}{dt} = -\bar{k}_0 C_A e^{-\frac{E}{RT}} - \Delta k_0 C_A e^{-\frac{E}{RT}} + \frac{q}{V}(C_{in} - C_A) \tag{94}$$

$$\frac{dT}{dt} = -\frac{\Delta H}{\rho C_p}\bar{k}_0 C_A e^{-\frac{E}{RT}} - \frac{\Delta H}{\rho C_p}\Delta k_0 C_A e^{-\frac{E}{RT}} + \frac{q}{V}(T_{in} - T) + \frac{hA}{\rho C_p V}(T_w - T) \tag{95}$$

At this point we consider an asymptotic observer for estimating the value of $C_A$ that appears in the regressor (i.e. the multiplicative term) of $\Delta k_0$. Its introduction is fully motivated by the theoretical analysis that will be performed below. The adaptive observer is then equal to:

$$\frac{d\hat{C}_A}{dt} = -\bar{k}_0 \hat{C}_A e^{-\frac{E}{RT}} + \frac{q}{V}\left(\hat{C}_{in} - C_A\right) - C_{Ae} e^{-\frac{E}{RT}}\widehat{\Delta k_0} + K_1\left(T - \hat{T}\right) \tag{96}$$

$$\frac{d\hat{T}}{dt} = -\frac{\Delta H}{\rho C_p}\bar{k}_0 \hat{C}_A e^{-\frac{E}{RT}} + \frac{q}{V}(T_{in} - T) + \frac{hA}{\rho C_p V} \times (T_w - T) - \frac{\Delta H}{\rho C_p} C_{Ae} e^{-\frac{E}{RT}}\widehat{\Delta k_0} + K_2\left(T - \hat{T}\right) \tag{97}$$

$$\frac{d\widehat{\Delta k_0}}{dt} = K_3\left(T - \hat{T}\right) \tag{98}$$

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

$$e_C = C_A - \hat{C}_A, e_T = T - \hat{T}, e_{k_0} = \Delta k_0 - \widehat{\Delta} k_0 \tag{99}$$

these are written as follows:

$$\frac{de}{dt} = Ae + Be_{Ce} \tag{100}$$

with:

$$A = \begin{bmatrix} -\frac{q}{V} - a_1 & -K_1 & -C_{Ae}e^{-\frac{E}{RT}} \\ a_1 a_2 & -K_2 & a_2 C_{Ae} e^{-\frac{E}{RT}} \\ 0 & -K_3 & 0 \end{bmatrix}, \quad e = \begin{bmatrix} e_C \\ e_T \\ e_{k_0} \end{bmatrix},$$

$$B = \begin{bmatrix} -\Delta k_0 e^{-\frac{E}{RT}} \\ a_2 \Delta k_0 e^{-\frac{E}{RT}} \\ 0 \end{bmatrix}$$

$$e_{Ce} = C_A - C_{Ae}, \quad a_1 = k_0 e^{-\frac{E}{RT}}, a_2 = -\frac{\Delta H}{\rho C_p}$$

From the theory of the asymptotic observers, we know that $e_{Ce}$ will tend asymptotically to zero: $\lim_{t\to\infty} e_{Ce} = 0$. We also know [3] that the matrix $B$ is bounded. Similarly, if $K_1$, $K_2$ and $K_3$ are bounded, then $A$ is bounded. Therefore the error dynamics are a time-varying system with an input converging asymptotically to zero. If the state matrix A is asymptotically stable, we can use a classical stability result (e.g. [49], 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:

$$\lambda^3 + \lambda^2\left(K_2 + a_1 + \frac{q}{V}\right) + \lambda\left(K_1 a_1 a_2 + K_2\left(a_1 + \frac{q}{V}\right) + K_3 a_2 C_{Ae} e^{-\frac{E}{RT}}\right) + K_3 \frac{q}{V} a_2 C_{Ae} e^{-\frac{E}{RT}} \tag{101}$$

It is then routine to check that $A$ is asymptotically stable via a proper choice of the gains $K_1$, $K_2$, and $K_3$, e.g. if we assign the dynamics of the observer with the following three eigenvalues $\lambda_1$, $\lambda_2$, $\lambda_3$. Fig. 4 illustrates the performance of the observer under the same initial and operating conditions as in Fig. 3, but with a 10% error on $k_0$. The gains have been chosen to assign the dynamics with

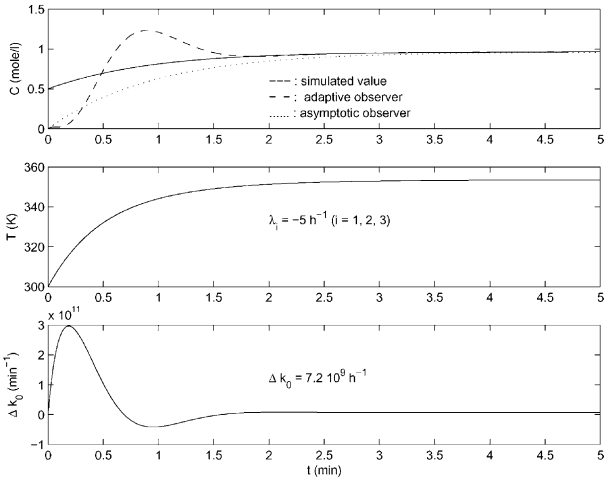


Fig. 4. Adaptive observer (initial transient).

$\lambda_1 = \lambda_2 = \lambda_3 = -5$. As before, the initial estimates of $C$ have been set to zero ($\hat{C}$ (adaptive observer) $= C_e$ (asymptotic observer) $= 0$ mole/l), while the initial temperature estimate has been initialized at the correct temperature value [$T(0) = T(0)$]. The unknown parameter $\hat{k}_0$ has been initialized at zero ($\hat{k}_0 = 0$ min$^{-1}$). 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 worth noting that the estimation of the temperature $T$ cannot be distinguished from the simulated value of $T$.

#### 4.3.1. Generalization

The generalization of both proposed observers in Sections 4.3 and 4.4 is based on the General Dynamical Model (49). If we consider that the measured outputs $y$ are process components (i.e. entries of the state vector $x$) (with possibly the temperature), then the part of the General Dynamical Model associated to $y$ is written as follows:

$$\frac{dy}{dt} = Y_y r - \frac{q}{V} y + F_y - Q_y + U_y \tag{102}$$

where $Y_y$, $F_y$, $Q_y$ and $U_y$ gather the rows of $Y$, $F$, $Q$ 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 $Y_y$ is full rank). The important step in the generalization consists then of introducing the following state transformation [42] (see also Section 5):

$$\zeta = Y_y^{-1} y \tag{103}$$

This transformation decouples all the kinetic terms and associates each of them to only one entry of the vector $\zeta$. Indeed Eq. (102) is rewritten as follows:

$$\frac{d\zeta}{dt} = -\frac{q}{V}\zeta + r + Y_y^{-1}\left(F_y - Q_y + U_y\right) \tag{104}$$

It is then straightforward to extend the design of both observers introduced in Sections 4.3 and 4.4 to each decoupled system ($\zeta_i$, $r_i$).

## 5. Comparison of the different state observers

In the preceding sections, 8 different observers have been presented: ELO, EKO, a nonlinear observer, asymptotic observer, interval observer, EKO for combined state and parameter estimation, observer with unknown parameter as design parameter, adaptive observer. Although there are other state observer schemes in the scientific literature, this gives an idea of the large diversity of state estimators available "on the market". The objective of the present section is to summarize as brie°y as possible the key features, the advantages and the drawbacks of the 8 state observers presented here.

The ELO and EKO are still to be considered as the basis for observer design. Their implementation will be successful if the process dynamics are (almost) exactly described by the model equations, and if the observers are initialized close enough to the true states since the gains are selected on the basis of the linearized tangent model of the observation error system (but this intialization is usually not a major issue in practice). The EKO presents the advantage of being an optimal solution with respect to a criterion that minimizes the observation error, but at the price of a higher complexity (since you have to integrate the gain equations). However once the process model is "moving away" from the true process dynamics, the ELO and EKO will fail to provide correct state estimates, as it has been illustrated in Section 2.4. Finally note that arbitrary fast convergence is possible only if the linearized tangent model is observable.

The nonlinear observer has typically similar advantages and drawbacks. If you consider the stability theoretical result in Section 2.3, it is worth noting that the observation error can be small if high gain values are selected (but high gains may generate large oscillations/variations in presence of noisy data). If the observation errors are potentially asymptotically small, these errors are related to the states of the transformed system equations, not to the original "physical" states. In our non-isothermal reactor example, this means that the estimate of the reactant concentration $C$ will be obtained by inverting the expression of $\phi$: any error in the model equations will result in wrong state estimation.

The asymptotic observer present the major advantage that convergence of the state estimation is guaranteed whatever the kinetics. All is needed is a correct reaction scheme (with known stoichiometric coefficients) and a correct heat balance (for non-isothermal processes). The price to pay is possibly the number of measured variables needed (one per reaction) and also the rate of convergence which is fixed by the operating conditions (no convergence is guaranteed in particular in batch reactors).

The interval observer explicitly integrates uncertainty bounds on process inputs and provides explicit bounds for the state estimates. Yet the results as presented here may appear rather conservative if the bounds have been selected large enough to integrate the worst uncertainties. However it is worth noting that recent developments in interval observers suggest that these problems can be eliminated in some instances, e.g. in presence of parameter uncertainty (see e.g. [44]).

The EKO for combined parameter and state estimation clearly presents the advantage that its design follows a standard and well-known line of reasoning. It is an a priori appealing solution in presence of parameter

uncertainty. However the tuning appears to be easily very complex, as it has been pointed in Section 4.2.

The observer with unknown parameter as design parameter certainly presents the appealing advantage that if the model structure is correct but with uncertain parameter values, the use of one uncertain parameter as design parameter will lead to unbiased state observation in steady-state. It is worth noting that this works even if other kinetic parameters have wrong values (e.g. $k_0$ in the numerical example of Fig. 4). However the limitation of the present observer is the transient behaviour: this is certainly a major drawback, e.g. for batch and fed-batch processes.

The adaptive observer presented here is indeed one particular adaptive observer. Its design is a response to the low applicability of "classical" adaptive observers. Indeed the design of adaptive observers has generated a large research activity in the eighties, but they were typically very difficult to tune and few applications resulted. If the design conditions are limited to systems affine in the parameters, it appears that the proposed adaptive observer is capable of handling nonlinear uncertainties. This is illustrated in Fig. 5, which presents a numerical simulation of the adaptive observer (96), (97) and (98) performed under the same initial conditions as in Fig. 4 and with a square wave of the inlet concentration $C_{in}$ (variations between 1 and 1.5 mol/l), but with a 10% error on $E$.

Finally note that the asymptotic observer, the interval observer, the observer with unknown parameter as design parameter, and the adaptive observer handle properly uncertainty on the kinetics. If other model parameters (e.g. yield coefficients in bioprocesses, or the heat of reaction in non-isothermal processes) are uncertain, biased estimation will result.

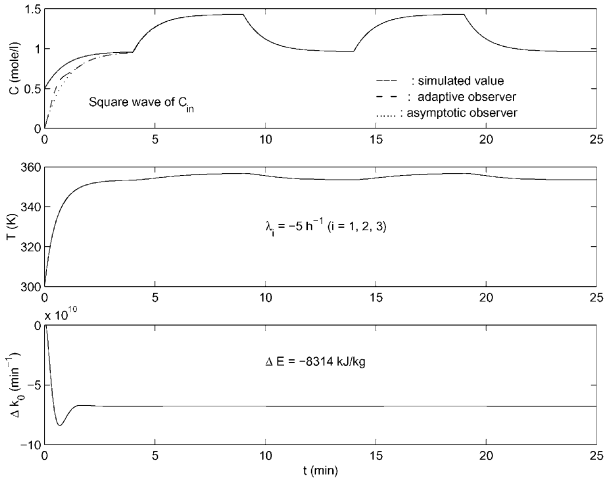


Fig. 5. Adaptive observer (10% error on E).

## 6. Decoupled parameter estimation

We have seen in the previous section how to combine state and parameter estimation in the same algorithm. But as already suggested in Section 4.2, improved estimation performances can possibly be expected if the state estimation and the parameter estimation are decoupled from each other. In this section, an estimation algorithm that allows this decoupling is presented: the observer-based estimator.

Consider that the process dynamics are described by the following equations:

$$\frac{dx}{dt} = F_1(x,u)\theta + F_2(x,u) \tag{105}$$

where $x$ is the state vector ($\dim(x)=p$), $\theta$ is the vector of (unknown) parameters ($\dim(\theta)=p$), and $F_1(x)$ and $F_2(x)$ are (matrix), generally nonlinear, functions of the state vector $x$. For example, if we rewrite the reaction rate $r(x)$ as the product of a function of the state and the unknown parameter $\theta$ ($r(x)=G(x)\theta$ where $G(x)$ is a $pxp$ diagonal matrix), the general dynamical model (49) presented in Section 3.1 can be expressed as follows:

$$\frac{dx}{dt} = YG(x)\theta + F - Q - \frac{q}{V}x \tag{106}$$

In the non-isothermal reactor example, a typical choice for $G(x)$ and $\theta$ would be: $G(x) = Ce^{-\frac{E}{RT}}, \theta = k_0$.

Assume that:

- **H1**. the $p$ parameters $\theta$ are unknown and possibly time-varying (with bounded time variations $\left\|\frac{d\theta}{dt}\right\| < M_1$);
- **H2**. at least $p$ state variables are available for on-line measurement.

From the assumption **H2**, we can define a state partition:

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \tag{107}$$

with $x_1$ $p$ measured variables, and $x_2$ the other ones (that can be measured or unmeasured). The dynamical equations can then be rewritten as follows:

$$\frac{dx_1}{dt} = F_{11}(x)\theta + F_{21}(x) \tag{108}$$

$$\frac{dx_2}{dt} = F_{12}(x)\theta + F_{22}(x) \tag{109}$$

Further assume that:

- **H3**. can be written as the product of two pxp matrices: $F_{11} = F_3F_4(x)$ with $F_4$ a diagonal matrix ($F_4 = \text{diag}\ \{f_{4,i}\}$, i = 1 to $p$) and $F_3$ being full rank for all admissible values of $x$ (for

(bio)chemical processes for instance, only positive values of the state variables (i.e. concentrations and possibly temperature) are considered);
- **H4**. $F_{11}(x)$ and $F_{21}(x)$ are known functions of $x$.

Under assumption **H3**, it may be possible to build an asymptotic observer to reconstruct the time evolution of $x_2$ independently of the unknown parameters $\theta$. In the following we consider that states included in $x_2$ are either accessible for on-line measurement or available via such observers, or that the dynamics of $x_1$ are independent of $x_2$.

In the context of stirred tank reactors (STR's),

$$F_3 = Y_1, \quad F_4 = G(x) \tag{110}$$

with $Y_1$ the yield coefficient matrix associated to $x_1$. Note that by constructing and assuming **H2**, the matrix $G(x)$ is a $pxp$ matrix. Assumption **H4** then means that the feedrates $F_1$ (associated to $x_1$), the gaseous outflow rates $Q_1$ (associated to $x_1$), the influent flow rate $q$ and the volume $V$ are known (via on-line measurements or user's choice), as well as the stoichiometric (yield) coefficients in $Y_1$ and the function $G(x)$.

The design of the observer-based estimator is based on Eq. (108) and follows indeed the line of reasoning for the design of Luenberger observers. This gives the following estimator equations:

$$\frac{d\hat{x}_1}{dt} = F_{11}(x)\hat{\theta} + F_{21}(x) - \Omega(x_1 - \hat{x}_1) \tag{111}$$

$$\frac{d\hat{\theta}}{dt} = [F_{11}(x)]^T \Gamma(x_1 - \hat{x}_1) \tag{112}$$

The basic motivation for the above structure for the estimator is the following. Like in a classical observer, the estimator equations are the combination of the process model $[F_{11}(x)\hat{\theta} + F_{21}(x)]$ and correction terms $[-\Omega(x_1 - \hat{x}_1)]$ and $\left[F_{11}(x)^T \Gamma(x_1 - \hat{x}_1)\right]$ on the measured variables. In the above observer-based estimator, the parameters $\theta$ are assimilated as states without dynamics. The weighting factor $[F_{11}(x)]^T$ in Eq. (112) is indeed the term multiplying the unknown parameters in the model equation: its introduction in the estimator equation derives from classical estimator design (e.g. [27]) and it is usually called the regressor. An important difference with respect to the extended Luenberger or Kalman observers is that the measured variables do not appear as estimates in the observer equations but with their "true" (measured) values.

The theoretical stability analysis of the above observer-based estimator is available in Ref. [3]: the main requirements are the negative definiteness of $\Omega^T\Gamma + \Gamma\Omega$ and the persistence of excitation of $F_{11}(x)$. However, its tuning may be difficult and intricate in practice, because of the close interaction of the unknown parameters in the estimator equations, and because its dynamics depends on the process variables. The latter may be of minor importance if the system is operated around a steady-state, but it will become crucial if the system covers a large range of operating conditions (as for fed-batch and batch reactors, or process start-ups and grade changes) possibly with large variations of the state variables, and as a consequence, the matrix $F_{11}(x)$. Good tracking capabilities of the parameters' variations are particularly essential in these circumstances. However, in the above form [(111),(112)] of the observer-based estimator, tuning may give very conservative values for the design parameters $\Gamma$ and $\Omega$, and result in bad tracking performance in some of the operating regions.

The above objectives for the tuning of the observer-based estimator can be achieved by considering first the following two steps in the reformulation of the algorithm:

(1) A state transformation;
(2) The re-arrangement of the estimator state vector entries.

Consider the following state transformation [the same as Eq. (103)]:

$$z = F_3^{-1} x \tag{113}$$

Then the dynamic equations of the system can be rewritten as follows:

$$\frac{dz}{dt} = F_4(x)\theta + F_3^{-1}F_{21}(x) \tag{114}$$

Due to the above transformation, only one state variable is associated with each unknown parameter $\theta$. In the specific case of stirred tank reactors, the invertibility of $F_3$ $(= Y_1)$ results from the independence of the p reactions and of the $p$ measured variables, as already mentioned before. The observer-based estimator can now be re-designed on the basis of Eq. (114):

$$\frac{d\hat{z}}{dt} = F_4(x)\hat{\theta} + F_3^{-1}F_{21}(x) - \Omega(z - \hat{z}) \tag{115}$$

$$\frac{d\hat{\theta}}{dt} = \Gamma(z - \hat{z}) \tag{116}$$

Due to the transformation (113), the observer-based estimator is now reformulated in a decoupled format for the unknown parameters $\theta_i$ (i = *1* to $p$). Because of the decoupled estimation formulation, an obvious choice for the matrices $\Omega$ and $\Gamma$ are diagonal matrices:

$$\Omega = \mathrm{diag}\{-\omega_i\}, \quad \Gamma = \mathrm{diag}\{\gamma_i\}, \quad \omega_i > 0, \quad \gamma_i > 0, \quad i = 1 \text{ to } p \tag{117}$$

In the above formulation of the estimation scheme, we have removed the regressor term $F_4(x)$ [$G(x)$ in the STR example] from the estimation equation of $\theta$ (116): since one of its main role is to explicitly transfer the coupling between the unknown parameters and the measured variables, its presence is not anymore essential.

The final step before the formulation of the tuning rule consists of a rearrangement of the estimator's equations. Let us gather each variable $z_i$ with its related parameter $\theta_i$ and re-arrange the entries of the vector $[z, \theta]^T$ in the following order in a vector $\zeta$:

$$\zeta = \begin{bmatrix} z_1 \\ \theta_1 \\ z_2 \\ \theta_2 \\ \cdots \\ z_p \\ \theta_p \end{bmatrix} \tag{118}$$

Let us first define the estimation error:

$$e = \zeta - \hat{\zeta} \tag{119}$$

The estimation error dynamics are readily derived from Eqs. (114), (115) and (116):

$$\frac{de}{dt} = Ae + b \tag{120}$$

with a block diagonal matrix $A$ with 2×2 blocks:

$$A = \mathrm{diag}\{A_i\}, \quad A_i = \begin{bmatrix} -\omega_i & f_{4,i}(x) \\ -\gamma_i & 0 \end{bmatrix}, \quad i = 1 \text{ to } p \tag{121}$$

and $b$ equal to:

$$b = \begin{bmatrix} 0 \\ \frac{d\theta_1}{dt} \\ 0 \\ \frac{d\theta_2}{dt} \\ \cdots \\ 0 \\ \frac{d\theta_p}{dt} \end{bmatrix} \tag{122}$$

The characteristic equation of the matrix $A$, $\det(\lambda I - A)$, is equal to:

$$\det(\lambda I - A) = \prod_{i=1}^{p} \left(\lambda^2 + \omega_i \lambda + \gamma_i f_{4,1}(x)\right) \tag{123}$$

The key idea of the tuning rule consists of choosing each $\gamma_i$ inversely proportional to the corresponding term $f_{4,i}(x)$:

$$\gamma_i = \frac{\bar{\gamma}_i}{f_{4,i}(x)}, \ \bar{\gamma}_i > 0, \quad i = 1 \text{ to } p \tag{124}$$

With the choice above, the characteristic equation (123) is rewritten as follows:

$$\det(\lambda I - A) = \prod_{i=1}^{p} \left(\lambda^2 + \omega_i \lambda + \bar{\gamma}_i\right) \tag{125}$$

and the observer-based estimator dynamics are now independent of the state variables. Such a choice corresponds to a Lyapunov transformation [41]. It is obviously valid for values of $f_{4,i}(x) \neq 0$: this condition is usually met easily in (bio)process applications, as will be illustrated in the following section.

The values of the design parameters can then be set to arbitrarily fix the estimator's dynamics for each unknown parameter $\theta_i$. Since the estimator reduces via the transformations to a set of independent second-order linear systems, the classical rules for assigning the dynamics of second-order linear systems apply straightforwardly here. The reader is therefore referred to the classical automatic control textbooks for further information on the subject. However the following basic guidelines are suggested.

One important guideline is to choose real poles:

$$\omega_i^2 - 4\bar{\gamma}_i \geqslant 0 \tag{126}$$

The objective is then to avoid inducing oscillations in the estimation of the parameters that do not correspond to any physical phenomenon related to the estimated reaction rates. Pomerleau and Perrier [43] suggest choosing double poles, i.e.:

$$\bar{\gamma}_i = \frac{\omega_i^2}{4} \tag{127}$$

The tuning of the estimation algorithm reduces then to the choice of one design parameter, $\omega_i$, per estimated parameter. This allows to have a design procedure that has the double advantage of being simple (one design parameter) and flexible (each parameter estimation can be tuned differently if needed, e.g. if the time variations of the parameters are different).

## 7. Real-life results

Two examples of real-life results of two of the methodologies developed above are presented here, i.e. the application of the asymptotic observer (Section 3.1) to an anaerobic digestion process, and the application of the observer-based estimator (Section 6) to animal cell culture.

Fig. 6 shows the estimation results for a pilot reactor of anaerobic digestion of 1 $m^3$ located in Narbonne (LBE-INRA) [5]. The asymptotic observer gives estimates of bicarbonate $B$, organic matter $S_1$ and volatile fatty acids $S_2$ (the 3 figures on the bottom right where the straight line (-) hold for the measured values used

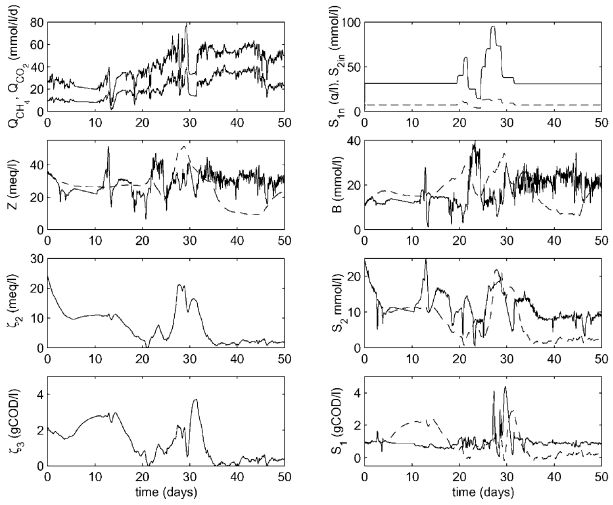


Fig. 6. Experimental results of an asymptotic observer applied to a pilot anaerobic digester.

for validation and the dotted lines (- -) hold for the estimates) on the basis of measurements of pH, gaseous outflow rates of $CH_4$ and $CO_2$, and influent concentrations $S_{1,in}$ (straight line ) and $S_{2,in}$ (dotted line) (the two figures on the top). The 3 figures on the bottom left represent the auxiliary variables of the asymptotic observer [The first one (Z) represents the total alkalinity for which there exists a "measured" value (in straight line) as the sum of bicarbonate $B$ and volatile fatty acids $S_2$]. Here the estimation task is particularly challenging due to the high complexity of the process dynamics (simply described by two reactions for the asymptotic observer design) and the large uncertainty not only of the process kinetics but also on the measurements of the influent.

As a second application, let us show real-life results of the observer-based estimator implemented on a 22 L pilot-scale bioreactor used for animal cell culture to estimate two specific growth rates $\mu_R$ (oxidation) and $\mu_F$ (glycolysis) [45]. Fig. 7 presents one set of experimental results. The glucose (Fig. 7a) and lactate (Fig. 7b) are measured via a FIA (Flow Injection Analysis) biosensor device. During this experiment, glucose was controlled via an adaptive linearizing controller to a low value equal to 1 mM. Because of the lack of reliable specific growth rate models, the validation of the estimation is performed by biomass concentration data: Fig. 7e compares the off-line data of biomass (o) with the estimation $X_v$ (dotted line) of biomass based on its mass balance equation and reconstructed from the on-line estimates of the specific growth rates $\hat{\mu}_R$ and $\hat{\mu}_F$:

$$\frac{dX_v}{dt} = \hat{\mu}_R X_v + \hat{\mu}_F X_v - \frac{q}{V} X_v \tag{128}$$

Note that the observer-based estimator detects the decrease of lactate around time = 120 h and gives a negative value to $\hat{\mu}_F$. Note also that the fact that the estimation of $\mu_R$ is pushed to negative values at the beginning of the culture is largely due to the measurement noise.

The selection of the design parameters values has typically followed the procedure described in Section 6. Numerical simulations have been used to give the first initial guesses based on the plausible measurement noise and specific growth rate model, then they have been adjusted in order to obtain the best validation possible with the biomass experimental data.

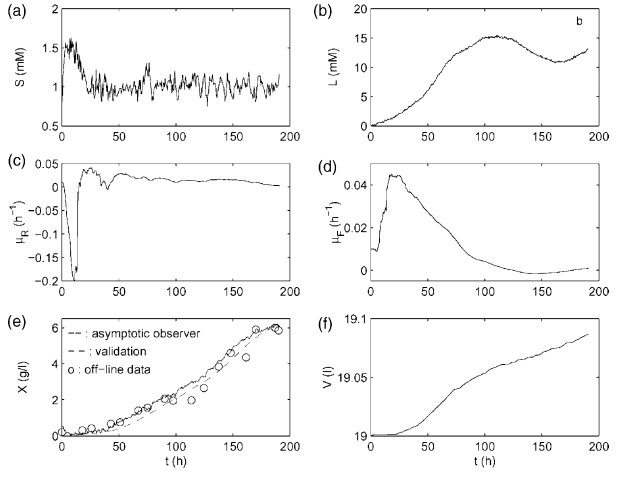


Fig. 7. Observer-based estimator: experimental results on an animal cell culture.

## 8. Challenges for the design of observers applied to batch processes

The design and application of state observers and parameter estimators to batch processes poses specific challenging questions, typically related to the time limitation of the batch operation. The question has been largely discussed in Ref. [1].[4]

One specific challenge of state observation and parameter estimation in batch processes is to design algorithms that are able to provide reliable estimates very quickly after the beginning of the batch. The problem is that so far the performance of parameter and state estimators are basically analyzed on the basis of the asymptotic behaviour of the related algorithms.

Bonvin and his coworkers [1,2,15] have identified several factors for the limitation of the extended Kalman filter when it is used to estimate both state variables and process parameters. These factors that are closely related to the inherent linearization of the estimator, are the following ones:

[4] It is obviously closely related to the control of the process, which is basically a finite-time optimal control problem, as it is nicely explained in Ref. [7].

(1) the poor knowledge about the key reaction parameters (these must be usually estimated, often with poor initial guesses);
(2) the large variations of the operating conditions (particularly in batch), making the use of simple linear approximations inappropriate;
(3) the inaccuracy of the initial estimates of the state variables;
(4) the imprecise measurement of the amounts of added agents;
(5) the sensitivity of the reaction systems to trace certain species (e.g. impurities in polymerisation reactions)

These works suggest that, beyond the proposed improvements, there is room for developing new tools for the design and analysis of state observers that are better appropriate to the specific features of batch processes. So far the scientific literature seems to very silent to what is often mentioned as a key question in process control today.

An appealing approach, developed in particular in Refs. [6] and [7], is the batch to batch improvement of the estimation and control algorithms.

In Ref. [6], the emphasis is put on model-based iterative learning control. In this approach, Model Predictive Control (MPC) is applied for trajectory tracking on the basis of a dynamical model of the batch process obtained by identification of Finite Impulse response (FIR) models or of AutoRegressive models with eXogenous inputs (ARX). Regularization is used in order to reduce the large dimensionality of the identification. In order to limit the negative effect of regularization (biased estimates), regularization weights are considered.

A survey on optimal control in a large sense (the authors prefer the words "dynamic optimization") in batch processes is presented in Ref. [7]. The batch-to-batch improvement is presented in the context of measurement-based optimization (MBO). MBO can include in particular parameter and state estimation as well as model reffinement. Typically, when state and parameter estimation is considered, one of the techniques described before is used. Improvement of the performance of the estimation of state variables and parameter can be obtained by considering for instance the recommendations given by [1] and [15] and summarized here Refs. in Section 4.1.

Beside the batch-to-batch improvement idea, new avenues should be traced in the design of state and parameter estimators. One of the main problem in the design of the presently available techniques is that it is based on *asymptotic* properties of the algorithms. In other words, the key issue usually addressed in the design of state observers and parameter estimators is to guarantee that for a time sufficiently large (tending to infinity!), the estimates will converge to the true values or within a bounded area close to these. But this approach is obviously inappropriate in the context of batch and semi-batch processes where one cannot wait very long before obtaining reliable estimates. The need to have rapidly reliable estimates is a crucial issue in batch and semi-batch operation. One possible suggestion would be to use, in the selection of the design parameters, criteria like the ITAE (Integral of the Time-weighted Absolute Error) criterion:

$$\min_K \int_0^\infty t|e(t)|dt \tag{129}$$

(where $K$ and $e$ denote the design parameters and the estimation error, respectively) or other criteria that penalize remaining errors after a defined period of time.

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