State Observation of a Nonlinear System: Application to (Bio)chemical Processes

M. Farza
Laboratoire d'Automatique de Procédés L.A.P., I.S.M.R.A., Université de Caen, 6, Boulevard Maréchal Juin,
F-14050 Caen cedex, France

H. Hammouri, C. Jallut, and J. Lieto
Laboratoire d'Automatique et de Génie des Procédés L.A.G.E.P., CNRS UPRES-A Q 5007,
Université Claude Bernard Lyon I, ESCPE—Lyon, Bât. 308 G, 43 Bd du 11 Novembre 1918, 69622 Villeurbanne cedex, France

The design of simple nonlinear observer-based estimators for the on-line estimation of the reaction rates in chemical and biochemical processes is presented. The proposed estimators do not assume or require any model for the reaction kinetics and are very successful for accurately estimating these variables. They are first presented in a continuous-time version. Then, the stability and convergence of a discrete-time version, obtained by a direct forward Euler discretization of these estimators, are established. A main characteristic of these estimators lies in the easiness of their implementation and in particular their calibration. Indeed, their gain does not necessitate the resolution of any dynamical system and is explicitly given. Moreover, its tuning is reduced to the calibration of a single parameter, and this is true regardless of the number of reaction rates to be estimated. The performances of the proposed estimators are highlighted through experimental results dealing with biological and chemical reactions performed in stirred-tank reactors.

Introduction

The lack of cheap and reliable instrumentation for the on-line measurement of the relevant variables in many processes definitely constitutes a serious obstacle for the development of these processes. One way to overcome this problem is to use "software sensors." A software sensor can be described as the association between a sensor (hardware) and an estimator (software). The latter is an algorithm based on the dynamical model of the process and is used to estimate the unmeasured state variables and the unknown process parameters from the on-line measurements. Over the last two decades, there has been a growing and widespread development of software sensors for the estimation of the reaction rates inside chemical reactors by using calorimetry techniques (see, e.g., Jutan and Uppal, 1984; Cott and Macchietto, 1989; Bonvin et al., 1989; De Vallière and Bonvin, 1989, 1990; Schuler and Schmidt, 1992, 1993; De Buruaga et al., 1997) and inside biochemical reactors (see, e.g., Shimizu et al., 1989; Wang and Stephanopoulos, 1984; Bastin and Dochain, 1990). This is because these rates are very complex functions of the operating conditions and the state of the process. The analytical modeling of these functions is often cumbersome and still constitutes the subject of continuing and intensive investigation. As a result, their estimation saves chemical and bioengineers the trouble of choosing a particular model among the several ones described in the literature. Moreover, these estimates, which are interesting for on-line adaptive control schemes, can also be used for basic investigations of the process under consideration.

Many works in the development of software sensors for the estimation of the reaction rates are based on an extended Kalman filter (EKF) approach that generally leads to complex nonlinear algorithms. Moreover, it is well known that EKF may give biased estimates or even diverge if it is not well initialized. A brief discussion on the limitations of the EKF and the failure of its use in practical situations is reported in Dochain et al. (1992). Another approach, developed by Bastin and Dochain (1990), consists of estimating the

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Correspondence concerning this article should be addressed to H. Hammouri.

unavailable state variables and the kinetics involved using a two-step approach. In the first step, the unmeasured state variables are estimated through (asymptotic) observers that are designed without any knowledge of kinetics expressions. In the second step, the estimated variables are considered as real measurements. Consequently, all state variables are supposed to be available, and they are then used to on-line estimate kinetic rates. Although the corresponding estimators are easy to implement, their tuning remains difficult (see, e.g., Farza and Chéruy, 1994; Oliveira et al., 1996). Indeed, a Bastin and Dochain's estimator which uses N component concentrations for the estimation of M reaction rates, involves two N tuning parameters, which have to be calibrated using a trial-and-error approach. Furthermore, this estimator is only proved to be stable, that is, the estimation error remains bounded. However, the expression of the corresponding bound is not given. Consequently, the choice of the most suitable values or expressions for the tuning parameters, ensuring accurate estimates of the unknown parameters (i.e., a decay to zero of the estimation error), becomes tedious and cumbersome.

In the present article, we show how efficient estimators of the reaction rates, involved in chemical and biochemical reactors, can be designed in a systematic and rigorous way without any assumptions concerning the rate expressions. These estimators are firstly synthesized in a continuous-time version using a high gain approach (see, e.g., Bornard and Hammouri, 1991; Gauthier et al., 1992). Then, we show that under a mild assumption of the sampling time, the discrete-time version of these estimators, obtained by a simple forward Euler discretization, still works as an estimator for the reaction rates. A main characteristic of the proposed estimators lies in the ease with which they are implemented and in particular calibrated. Indeed, their tuning is reduced to the calibration of a single tuning parameter, and this is true whatever the number of components and reactions being considered.

An outline of this article is as follows: in the next section, we respectively introduce bioreactors and chemical-reactor state-space models, which are the basis of the reaction rate estimator's synthesis. In the third section, we show how one can design observers for a class of nonlinear systems that includes bioreactors and chemical-reactor models. These observers are proposed in a continuous as well as a discrete-time version. We then show in the fourth section how the proposed observers can be used for the on-line estimation of the reaction rates, and the equations of the corresponding estimators are given. Finally, in the fifth section we present two experimental results: the first deals with a batch process of lactic acid production, while the second concerns an esterification reaction held in a batch-fed reactor. In each case, the rates of the reactions involved are estimated through the proposed observers and the obtained results are presented.

Modeling of Chemical and Biochemical Reactors

A (chemical) biochemical process can be described by a set of N state variables, the component concentrations, $C_1, \ldots, C_N$, which interact through M (chemical) biochemical reactions $r_1, \ldots, r_M$. These, in general, occur in a stirred-tank reactor. The dynamical model of a biochemical process is very similar to that of the chemical one, the main difference being the explicit presence of the temperature in the state vector when considering the chemical process. Nevertheless, for both processes, the components' mass balances are often considered, and they can be written as follows:

$$\dot{C} = Yr - DC + DC_{in} - G, \tag{1}$$

where

$C = (C, \ldots, C_N)^T$: vector of component concentrations $\in \mathbb{R}^N$
$C_{in} = (C_{in1}, \ldots, C_{inN})^T$: vector of influent component concentrations $\in \mathbb{R}^N$ $(\mathrm{g \cdot L^{-1}})$
$G = (G_1, \ldots, G_N)^T$: vector of normalized mass outflow rates in gaseous form $\in \mathbb{R}^N$ $(\mathrm{g \cdot L^{-1} \cdot s^{-1}})$
$Y = N \times M$ yield (stoichiometric) coefficients matrix
$r = (r_1, \ldots, r_M)^T$: vector of reaction rates $\in \mathbb{R}^M$ $(\mathrm{g \cdot L^{-1} \cdot s^{-1}})$
$D =$ dilution rate $\in \mathbb{R}$ $(\mathrm{s^{-1}})$.

For biochemical processes, the dynamical balance model is restricted to the system in Eq. 1. In the case of chemical ones, the energy balance is considered and the system in Eq. 1 is augmented by the following equation:

$$\dot{T}_R = -\frac{1}{\rho_R c_{pR}} \Delta H^T r - Q + D(T_{Rin} - T_R), \tag{2}$$

where

$T_R =$ temperature inside the reactor $\in \mathbb{R}$ (K)
$\Delta H^T = (\Delta H_1, \ldots, \Delta H_M)$: the vector of the reaction enthalpies $\in \mathbb{R}^M$ $(\mathrm{kJ \cdot g^{-1}})$
$T_{Rin} =$ inlet temperature $\in \mathbb{R}$ (K)
$\rho_R =$ density of the reaction bulk $\in \mathbb{R}$ $(\mathrm{g \cdot L^{-1}})$
$c_{pR} =$ specific heat of the reaction bulk $\in \mathbb{R}$ $(\mathrm{kJ \cdot g^{-1} \cdot K^{-1}})$
$Q =$ normalized heat flux $\in \mathbb{R}$ $(\mathrm{K \cdot s^{-1}})$.

In fact, the term Q is given by

$$Q = \frac{UA(T_R - T_j)}{\rho_R c_{pR} V_R}, \tag{3}$$

where U is the overall heat-transfer coefficient $(\mathrm{W \cdot m^{-2} \cdot K^{-1}})$, A is the heat-transfer surface area $(\mathrm{m^2})$, T_j is the coolant/heating fluid temperature (K), and V_R is the reactor volume (L). The mathematical model of chemical reactors can also be extended to account for the dynamics of T_j. In the case of a cooling/heating fluid flowing through the jacket, this dynamics can be described by the following energy balance equation:

$$\dot{T}_j = \frac{UA}{\rho_j c_{pj} V_j}(T_R - T_j) + \frac{F_j}{V_j}(T_{jin} - T_j), \tag{4}$$

where ρ_j $(\mathrm{g \cdot L^{-1}})$, c_{pj} $(\mathrm{kJ \cdot g^{-1} \cdot K^{-1}})$, and V_j (L), respectively, denote the density, the specific heat, and the volume of the cooling/heating fluid; F_j $(\mathrm{L \cdot s^{-1}})$ is the coolant/heating fluid flow rate; and T_{jin} (K) is its inlet temperature.

In the sequel, we suppose that the dynamical model of the chemical reactors is described by Eqs. 1 and 2 only.

In the case of bioprocesses, the vector of reaction rates r is often split into the product of two terms:

$$r = H(C)\alpha(C),$$

where each element of the vector α is called the "specific reaction rate," and H is an $M \times M$ state-dependent diagonal matrix whose elements correspond to the reactants. The expression of each diagonal element $h_j(C)$ of the matrix H is

$$h_j(C) = \left(\prod_{n \sim j} C_n \right). \tag{5}$$

The notation $n \sim j$ means that the multiplication $\prod$ is taken over the components C_n, which are reactants in the reaction r_j (including the autocatalysts). The preceding minimal modeling of the reaction rates is in accordance with practice, and it is based on the following fact: a reaction can take place only if all the involved reactants (including autocatalysts) are present in the reactor. Otherwise, the reaction rate is necessarily zero. For example, in the case of a simple growth reaction involving a single biomass X that is grown on a single substrate S, the rate of the growth reaction r can be written as follows:

$$r = XS\alpha(X,S),$$

where α is the specific reaction rate. The usual approach adopted in fermentation modeling consists of writing the growth rate in the following form:

$$r = \mu(X,S)X,$$

where μ is the specific growth rate. Several possible expressions for μ have been reported in the literature (see, e.g., Frederickson and Tsuchiya, 1977). The most famous is undoubtedly Monod's law:

$$\mu = \frac{\mu_{\max} S}{K_S + S},$$

where $\mu_{\max}$ is the maximum specific growth rate, and K_S is the saturation constant. According to Monod's law, the expression of the specific reaction rate α is then

$$\alpha(X,S) \triangleq \alpha(S) = \frac{\mu_{\max}}{K_S + S}.$$

As in bioreactors, the reaction rates r_j, $j = 1, \ldots, M$, in chemical reactors are generally nonlinear functions of the state of the process. The vector r can be written as follows:

$$r = H(C)\alpha(T_R),$$

where H is an $M \times M$ diagonal matrix and α is an M dimensional vector. Each diagonal term of the matrix H is (generally) a nonlinear function of C. For example, in the case where the process kinetics obeys the Arrhenius law, each reaction rate r_j specializes as follows:

$$r_j = k_{0j}\varphi_j(C)e^{-E_j/RT_R},$$

where k_{0j} is the reaction-rate constant, E_j is the activation energy, R is the ideal-gas constant, and φ is generally a nonlinear function of the reactant concentrations. In such a case, the diagonal term h_j of H and the jth component α_j of α are

$$h_j(C) = k_{0j}\varphi_j(C) \quad \text{and} \quad \alpha_j(T_R) = e^{-E_j/RT_R}.$$

In the sequel and other processes, we do not assume any model for the reaction rates r_j. As a result, the following system can be adopted as a unified modeling framework for chemical and biochemical reactors:

$$\dot{\xi} = Kr - D\xi + W, \tag{6}$$

with

$$\xi \triangleq \begin{pmatrix} T_R \\ C \end{pmatrix}; \quad K \triangleq \begin{pmatrix} -\dfrac{\Delta H^T}{\rho_R c_{pR}} \\ Y \end{pmatrix}$$

and

$$W = \begin{pmatrix} DT_{Rin} - Q \\ DC_{in} - G \end{pmatrix}$$

for chemical reactors, and

$$\xi \triangleq C; \quad K \triangleq Y \quad \text{and} \quad W \triangleq DC_{in} - G$$

for bioreactors.

As previously mentioned, the modeling of r is a difficult and hazardous task. In order to overcome these difficulties, we propose nonlinear observers for the on-line estimation of these variables. The approach to design estimators for the reaction rates is not new and has often been exploited (Wang and Stephanopoulos, 1984; Shimizu et al., 1989; Bastin and Dochain, 1990): it consists of augmenting the state vector to include, in addition to the state variables, those of the process parameters that it is not desirable for models to express, that is, the reaction rates. As no balances are available for these kinetics, however, we will assume that their dynamics are described by unknown and bounded functions. Obviously, such a hypothesis is reasonable and is in accordance with practical situations.

We now introduce a simple partition in order to exhibit a subsystem of the system in Eq. 6, which will be the basis of the design of the estimator of the reaction rates. For this purpose, we note that, in most practical situations, the number of reactions is lower than or equal to the number of components. Moreover, the matrix K is usually of full rank. Therefore, we assume the following conditions:

(C1) K, D, W are known.

(C2) The temperature T_R is supposed to be measured when chemical reactors are considered.

(C3) If ξ is partitioned into the sets of measured variables $\xi^{(1)}$ and nonmeasured variables $\xi^{(2)}$: $\xi = \begin{pmatrix} \xi^{(1)} \\ \xi^{(2)} \end{pmatrix}$ and accordingly, $K = \begin{pmatrix} K^{(1)} \\ K^{(2)} \end{pmatrix}$, then we have $rank(K^{(1)}) = rank(K) = M$.

Note that condition C3 implies that the number of measured components is greater than or equal to the number of reactions in the case of bioreactors, and it is greater than or equal to the number of reactions minus one when chemical reactors are considered. For the latter, the set of measured variables is constituted by the temperature and at least $(M-1)$ component concentrations.

In the sequel, we shall adopt the following unifying (but not simplifying) theory for modeling the reaction rates:

$$r(t) = H(\xi^{(1)})\,\alpha(t).$$

Such a theory only means that the vector of reaction rates r is factored under the product of a completely unknown time-varying vector α and an $M \times M$ known diagonal matrix H, that is, a diagonal matrix where each diagonal term is known either by measurement or by the user's choice. In the case where the vector of the reaction rates is completely unknown, we obviously have

$$H(\xi^{(1)}) \overset{\Delta}{=} I_M \qquad \text{and} \qquad \alpha(t) \overset{\Delta}{=} r(t),$$

where I_M denotes the $M \times M$ identity matrix.

The vector α will be referred to as the vector of the specific reaction rates, and our objective is to estimate these parameters.

According to condition (C3), one can find, after permutations of the rows of $K^{(1)}$ (if necessary), an $M \times M$ square submatrix K' of $K^{(1)}$, which is of full rank. Let K'' such that

$$K = \begin{pmatrix} K' \\ K'' \end{pmatrix}$$

up to rows permutation. The system in Eq. 6 can be rewritten as follows:

$$\begin{cases} \dot{\xi}' = K'H(\xi^{(1)})\,\alpha - D\xi' + W' \\ \dot{\xi}'' = K''H(\xi^{(1)})\,\alpha - D\xi'' + W'', \end{cases} \tag{7}$$

where

$$\begin{pmatrix} \xi' \\ \xi'' \end{pmatrix} \; and \; \begin{pmatrix} W' \\ W'' \end{pmatrix},$$

respectively, denote the partitions of ξ and W induced by the partition of K just given. Notice that all components of ξ' are measured, since ξ' is a subvector of $\xi^{(1)}$. Let s denote the remaining subvector, namely

$$\xi^{(1)} = \begin{pmatrix} \xi' \\ s \end{pmatrix}$$

up to rows permutation. For the estimation problem, we focus on the following reduced system:

$$\begin{cases} \dot{\xi}' = K'H(\xi', s)\,\alpha - D\xi' + W' \\ \dot{\alpha} = \epsilon(t) \\ y = \xi', \end{cases} \tag{8}$$

where ϵ is an unknown bounded function that may depend on the concentrations, the temperature, the inputs, the noise, and so forth. In the next section we propose state monitors for a class of nonlinear systems that includes the system in Eq. 8. Then we will show how such observers can use the measurements of ζ' to estimate the specific reaction-rate vector α.

Observer Design for a Class of Nonlinear Systems

Continuous version

Consider the following system:

$$\begin{cases} \dot{z}_1(t) = F_1(z_1(t), s(t))\,z_2(t) + b_1(u(t), z_1(t), s(t)) \\ \dot{z}_2(t) = b_2(u(t), z_1(t), s(t)) + \epsilon(t) \\ y(t) = z_1(t), \end{cases} \tag{9}$$

where the state

$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \in \mathbb{R}^{2n};\; z_1,\, z_2 \in \mathbb{R}^n;$$

the input $u \in \mathbb{R}^m$; the output $y \in \mathbb{R}^n$; $s \in \mathbb{R}^q$ is a known signal; F_1 is an $n \times n$ matrix, which is of class $\mathfrak{C}^1$ with respect to its arguments; and ϵ is an unknown function that may depend on z, s, u, noise, and so on. It is clear that the class of system in Eq. 9 includes that of the system in Eq. 8.

For $\epsilon = 0$, it is well known that the system in Eq. 9 includes an exponential observer if the following system is completely uniformly observable:

$$\begin{cases} \dot{\xi}_1 = F_1(y, s)\,\xi_2 \\ \dot{\xi}_2 = 0 \\ y = \xi_1, \end{cases}$$

with $(\xi_1, \xi_2) \in \mathbb{R}^n \times \mathbb{R}^n$ and (y, s) is the input signal. However, the gain of the observer is obtained through differential equations [Riccati differential equations or Lyapunov differential equations (see, for instance, Bornard et al., 1988; Hammouri and De Leon, 1991)]. We want to give an estimator whose gain is simple to calculate and that does not require the resolution of any dynamical system. We will show that the estimators we propose later are such that the estimation error converges exponentially to zero in the case where $\epsilon = 0$. If $\epsilon(t) \neq 0$ and is bounded, the estimation error lies in some ball $B(0, \rho(\delta))$, where $\delta = \sup_{t \geq 0} \|\epsilon(t)\|$ and $\lim_{\delta \to 0} \rho(\delta) = 0$.

The system in Eq. 9 can be written in the following condensed form:

$$\begin{cases} \dot{z} = F(z_1, s)\,z + B(u, z_1, s) + \bar{\epsilon}(t) \\ y = Cz, \end{cases} \tag{10}$$

where

$$F(z_1,s)=\begin{bmatrix} 0 & F_1(z_1,s) \\ 0 & 0 \end{bmatrix},$$

$$B(u,z_1,s)=\begin{bmatrix} b_1(u,z_1,s) \\ b_2(u,z_1,s) \end{bmatrix}, \qquad \bar{\epsilon}(t)=\begin{bmatrix} 0 \\ \epsilon(t) \end{bmatrix},$$

and $C=[I_n, 0]$, with I_n the $n\times n$ identity matrix.

We assume the following:

(A1) There exist finite real numbers α, β, with $0<\alpha\le\beta$ such that $\forall\xi\in\mathbb{R}^n$, $\forall t\ge 0$:

$$\alpha^2 I_n \le F_1^T(\xi, s(t))F_1(\xi, s(t)) \le \beta^2 I_n.$$

(A2) The function $\epsilon(t)$ is bounded.

(A3) The function $s(t)$ and its time derivative $(ds(t)/dt)$ is bounded.

(A4) B is global Lipschitz with respect to z_1, locally uniformly with respect to u and s, that is,

$$\forall\sigma,\sigma'>0; \qquad \exists\sigma''>0; \qquad \forall u,\ \|u\|\le\sigma;$$
$$\forall s,\ \|s\|\le\sigma'; \qquad \forall z_1\in R^n:\ \left\|\frac{\partial B}{\partial z_1}(u,z_1,s)\right\|<\sigma''.$$

(A5) F_1 is global Lipschitz with respect to z_1, locally uniformly with respect to s.

Notice that assumptions (A4) and (A5) can be omitted in the case where the trajectories of the system in Eq. 10 lie within a bounded set Ω. Indeed, in such a case, we can respectively extend the nonlinearities F and B into $\tilde{F}$ and $\tilde{B}$ in such a way that the restriction of $\tilde{F}$ and $\tilde{B}$ to Ω respectively coincide with F and B on Ω, and that $\tilde{F}$ and $\tilde{B}$ become global Lipschitz on the whole state space. These prolongation techniques were initially used by Bornard and Hammouri (1991) and Gauthier et al. (1992). In the sequel, we will not consider these prolongations for the following reasons:

- From a practical point of view, such techniques are rarely used.
- The methodology involves intricate manipulations that are not relevant in the context of this work.

Now consider the system given by

$$\dot{\hat{z}}=F(\hat{z}_1,s)\hat{z}+B(u,\hat{z}_1,s)-\Lambda^{-1}(\hat{z}_1,s)S_\theta^{-1}C^T(C\hat{z}-y), \quad (11)$$

where

(i) $\hat{z}=\begin{bmatrix}\hat{z}_1\\ \hat{z}_2\end{bmatrix}\in\mathbb{R}^{2n}$, $\hat{z}_1$, $\hat{z}_2\in\mathbb{R}^n$, and $(u,\ s)$ and y are, respectively, the input and the output of the system in Eq. 10.

(ii) $\Lambda(\hat{z}_1,\ s)=\begin{bmatrix} I_n & 0 \\ 0 & F_1(\hat{z}_1,s)\end{bmatrix}$.

(iii) S_θ is the unique symmetric positive definite matrix satisfying the algebraic Lyapunov equation

$$\theta S_\theta + A^T S_\theta + S_\theta A - C^T C = 0, \qquad (12)$$

where $A=\begin{bmatrix} 0 & I_n \\ 0 & 0\end{bmatrix}$ and $\theta>0$ is a parameter (see Gauthier et al., 1992).

We then state the following:

Theorem 1. Assume that the system in Eq. 10 satisfies Assumptions (A1) to (A5). Then, $\forall\sigma>0$; $\exists\theta_o>0$; $\forall\theta>\theta_0$; $\exists\lambda_\theta>0$; $\exists\mu_\theta>0$; $\exists M_\theta>0$; $\forall u$, $\|u\|_\infty\le\sigma$; $\forall\hat{z}(0)\in R^{2n}$; we have

$$\|\hat{z}(t)-z(t)\|\le\lambda_\theta e^{-\mu_\theta t}\|\hat{z}(0)-z(0)\|+M_\theta\delta,$$

where u is an admissible control, $\|u\|_\infty$ is its upper bound, $z(t)$ is the trajectory of Eq. 10 associated with the input u, $\hat{z}(t)$ is any trajectory of the system in Eq. 11 and δ is the upper bound of $\|\epsilon\|$. Moreover, we have $\lim_{\theta\to\infty}\mu_\theta=+\infty$ and $\lim_{\theta\to\infty}M_\theta=0$.

Proof. See Appendix A.

Remarks

1. Observe that when $\epsilon(t)=0$, the convergence of the estimation error is an exponential one. In the case where $\epsilon(t)\neq 0$, the asymptotic error can be made arbitrarily small by choosing sufficiently large values of θ. However, very large values of θ are to be avoided in practice, since the estimator may become noise sensitive. Thus, the choice of θ is a compromise between fast convergence and sensitivity to noise.

2. Note that the solution of Eq. 12 is given by

$$S_\theta=\begin{bmatrix} \frac{1}{\theta}I_n & -\frac{1}{\theta^2}I_n \\ -\frac{1}{\theta^2}I_n & \frac{2}{\theta^3}I_n \end{bmatrix},$$

and consequently the gain of estimator, Eq. 11, is

$$\Lambda^{-1}(\hat{z}_1,s)S_\theta^{-1}C^T=\begin{bmatrix} 2\theta I_n \\ \theta^2 F_1^{-1}(\hat{z}_1,s)\end{bmatrix}.$$

(3) Following the same approach as in the proof of Theorem 1, one can show that the state estimate $\hat{z}_1$ can be substituted by its measurements, y, in the equations of estimator, Eq. 11. As a result, Assumptions (A4) and (A5) are no longer necessary and estimator, Eq. 11, is replaced by the following one:

$$\dot{\hat{z}}=F(y,s)\hat{z}+B(u,y,s)-\Lambda^{-1}(y,s)S_\theta^{-1}C^T(C\hat{z}-y). \quad (13)$$

Equation 13 shall be referred to as an estimator up to output injection. We shall show below that the discrete version obtained by a direct forward Euler discretization of this estimator works as an estimator for the discrete version of the system in Eq. 10 (obtained by the same discretization).

Discrete version

The estimators previously given assume continuous time observations. Since this is rarely the case in bio- and chemical processes, we are encouraged to find a discrete counterpart for these algorithms. In fact, we shall show that under an additional assumption on the sampling time, a direct forward Euler discretization of the proposed estimators still works for the systems being considered. In order to have a realistic and moderate assumption of the sampling time, we deal here with the discretization of the continuous estimator up to output injection, that is, the system in Eq. 13. This is because the convergence of the discrete version resulting from the original continuous estimator—the system in Eq. 11—requires strong assumptions of the sampling time, which may not be verified for relatively high values of this parameter.

Consider the forward Euler discretization of the system in Eq. 9:

$$\begin{cases} z_{1(t+1)} = z_{1t} + T_s\left[F_1(z_{1t}, s_t)z_{2t} + b_1(u_t, z_{1t}, s_t)\right] \\ z_{2(t+1)} = z_{2t} + T_s\left[b_2(u_t, z_{1t}, s_t) + \epsilon_t\right] \\ y_t = z_{1t}, \end{cases} \tag{14}$$

where T_s is the sampling time; z_{1t}, z_{2t}, u_t, s_t, ϵ_t, and y_t are the corresponding values of $z_1(t)$, $z_2(t)$, $u(t)$, $s(t)$, $\epsilon(t)$, and $y(t)$ at the present sampling time; and $z_{1(t+1)}$ and $z_{2(t+1)}$, respectively, denote the values of $z_1(t)$ and $z_2(t)$ at the next sampling time.

The system in Eq. 14 can be written in the following condensed form:

$$\begin{cases} z_{t+1} = z_t + T_s\left[F(y_t, s_t)z_t + B(u_t, y_t, s_t) + \bar{\epsilon}_t\right] \\ y_t = z_{1t}. \end{cases} \tag{15}$$

Similarly, the forward Euler discretization of estimator, Eq. 13, is

$$\hat{z}_{t+1} = \hat{z}_t + T_s\Big[F(y_t, s_t)z_t + B(u_t, y_t, s_t) - \Lambda^{-1}(y_t, s_t)S_\theta^{-1}C^T(C\hat{z}_t - y_t)\Big]. \tag{16}$$

We suppose that the sampling time T_s is such that the following holds:

(A6) $\exists T_0 > 0$; $\forall T_s \in [0, T_0]$; $\exists \eta \in [0, 1]$; $\forall t$: $\| I_n - F_1(y_{t+1}, s_{t+1})F_1^{-1}(y_t, s_t)\| \le \eta$.

Notice that Assumption A6 is quite moderate, and is in particular satisfied for relatively small values of the sampling time T_s.

We now state the following theorem.

Theorem 2. Assume that the system in Eq. 15 satisfies Assumptions (A1), (A2), (A3), and (A6). Then, for every bounded input u, there exist $\theta_0 > 0$, $\theta_1 > 0$; for every $\theta \in [\theta_0, \theta_1]$; there exist $m_{1\theta} > 0$, $m_{2\theta} > 0$ and $d_\theta \in [0, 1]$ such that for every $t = 0, T_s, 2T_s, \ldots$, we have

$$\| \hat{z}_t - z_t \| \le m_{1\theta}(d_\theta)^t \| \hat{z}(0) - z(0) \| + m_{2\theta}\delta,$$

where δ is the upper bound of $\| \epsilon_t \|$.

Proof. See Appendix B.

Remarks

1. The tuning parameter θ cannot be taken arbitrarily large as in the continuous case. It is bounded on the top by $\theta_1 = 1/T_s$. In fact, values of θ such that θT_s is close to 1 are to be avoided, since the estimator may become noise sensitive. Here again, the choice of θ is a compromise between fast convergence and the estimator's noise sensitivity.

2. As in the continuous case, when $\epsilon_t = 0$, the convergence of the estimation error is exponential. When $\epsilon_t \neq 0$ and is bounded, the asymptotic error is smaller than a positive constant $m_{2\theta}\delta$.

3. As one would expect, the bounds of the estimation error are as small as δ and T_s (see proof).

4. It should be emphasized that for reasons of clarity the sampling time was assumed to be constant. Nevertheless, extension of the results to systems discretized with a variable step size can be adequately achieved.

Application to Chemical and Biochemical Reactors

As previously mentioned, it is easy to see that the system in Eq. 8 is less than Eq. 9. As a result, the estimators proposed in the previous section can be used for the on-line estimation of the reaction rates in bioreactors as well as in chemical reactors. However, before using these estimators, we discuss and check Assumption A1 to A5, after which we will write the equations of the corresponding estimators. The equations of physical systems (in particular the system in Eq. 8) make sense only on the physical, bounded domain Ω (i.e., the trajectories of the system in Eq. 8 lie inside Ω). On such a compact domain Ω, the right inequality of Assumption A1, as well as Assumptions A2 to A5 are satisfied. Let us now examine the left inequality of Assumption A1 (i.e., the lower bound of $F_1^TF_1$). This condition will be satisfied if each element of the diagonal matrix H remains bounded away from zero. Indeed, we have

$$(K'H)^T(K'H) = H^TK'^TK'H \ge a_1H^TH$$

for some $a_1 > 0$, since K' is of full rank. Now, we remind the reader that each term of H corresponds to the product of the reactant concentrations. Thus, the nullity of such a product means that the corresponding reaction no longer takes place in the reactor and the mathematical model has to be reconsidered. Because of this, it seems reasonable to assume that the elements of H remain bounded away from zero, with the result that Assumption A1 is satisfied. Moreover, as was previously mentioned, one can prolong the nonlinearities F_1 and B outside Ω in such a way that Assumptions A1, A4, and A5 are globally satisfied (see, e.g., Gauthier et al., 1992).

According to this, the nonlinear observer-based estimators given earlier can be used in order to estimate the reaction rates from the measurements of the components' concentrations. The equations of the continuous-time version of the corresponding estimator are

$$\begin{cases} \dot{\hat{\xi}}' = K'H(\hat{\xi}', s)\hat{\alpha} - D\hat{\xi}' + W' - 2\theta(\hat{\xi}' - \xi') \\ \dot{\hat{\alpha}} = -\theta^2\left(K'H(\hat{\xi}', s)\right)^{-1}(\hat{\xi}' - \xi'). \end{cases} \tag{17}$$

The discrete-time estimator is

$$\begin{cases} \hat{\xi}'_{t+1} = \hat{\xi}'_t + T_s\left[K'H(\xi'_t, s_t)\hat{\alpha}_t + - D\xi'_t + W'_t - 2\theta(\hat{\xi}'_t - \xi'_t)\right] \\ \hat{\alpha}_{t+1} = \hat{\alpha}_t - T_s\theta^2(K'H(\xi'_t, s_t))^{-1}(\hat{\xi}'_t - \xi'_t). \end{cases} \tag{18}$$

Remarks

1. We have assumed that the matrix K, and in particular the yield coefficient matrix Y, is known. In practice and par-

ticularly for bioreactors, this is not always the case, and in some instances, these coefficients may not be well known or may even be completely unknown and need to be estimated. In such a case, it suffices to consider the product of each unknown yield with the multiplying kinetic rate, as a new rate that needs to be estimated. The mathematical model resulting from this new reformulation is in general given by Eq. 9 and the estimators proposed can be used in order to jointly estimate the reaction rates and the unknown yield coefficients. In some cases, however, the matrix of known yield coefficients appearing in the resulting model does not remain invertible, in which case the estimators proposed in this section cannot be used. Such a situation always occurs when the number of unknown parameters (the reaction rates and unknown yield coefficients) is greater than the number of state variables.

2. We have assumed that the term Q is known for the chemical reactors. In some instances, such a hypothesis may not be satisfied in practice. Indeed, suppose that Q is modeled as in Eq. 3. Then, one has to know the value of UA in order to quantify Q. Similarly, the term $C_R = \rho_R c_{pR} V_R$ can vary in some processes, and it is desirable to obtain an on-line estimate of this parameter. For the purposes of this article, estimation of UA and C_R is not discussed here and will be treated elsewhere.

Experimental Results

In order to confirm and validate the preceding theoretical results, experimental studies were performed using a laboratory-scale fermentor and a reaction calorimeter. The concerned bioprocess deals with batch lactic acid production, while the chemical reaction is an esterification held in a fed-batch reactor. We propose to briefly describe these processes and present the estimation results of the corresponding reaction rates.

Estimation of the reaction rates of lactic acid production in a batch process

The relevant process deals with the production of lactic acid from lactose. The fermentation is performed in a 2-L stirred-tank reactor with controlled temperature ($T = 38$°C) and pH (pH = 6). The pH was set automatically by adding a $6N$ ammonia solution. The culture used is *Lactobacillus rhamnosus*.

The fermentation medium was composed of 100 g/L of ultrafiltered whey (in powder, which is equivalent to 80 g/L of pure lactose), 3 g/L yeast extract, 0.03 g/L $MnSO_4$, and 0.5 mL/L Tween 80. The medium was sterilized in the fermentor at 120°C for 20 min (Moueddeb, 1994).

The measurements of biomass, lactose, and lactic acid were performed as follows: the cell density was measured by optical absorbance at 570 nm after dilution. The biomass concentration was then deduced through a linear correlation between the absorbance and the dry weight; the lactose concentration was quantified using HPLC (Waters Associates, Milford, MA). The lactic acid was assayed by enzymatic analysis using a Y.S.I. 2000 apparatus (Bioblock, Vaulx Milieu, France).

The dynamical balance model of the process is written as follows:

$$\begin{cases} \dot{X} = r_1 \\ \dot{S} = -r_2 \\ \dot{P} = r_3, \end{cases} \tag{19}$$

where S, X, and P denote, respectively, the concentrations of lactose, *Lactobacillus rhamnosus*, and lactic acid; all these concentrations are measured. The terms r_1, r_2, and r_3 denote, respectively, biomass growth, substrate consumption, and product synthesis rates. In fact, the term r_1 also accounts for the decay phenomenon that may occur during the fermentation. For the sake for clarity, this will be referred to as the growth rate in the sequel. The rates r_1, r_2, and r_3 can be written as follows:

$$r_1 = \alpha_1 X \qquad r_2 = \alpha_2 X \qquad \text{and} \qquad r_3 = \alpha_3 X,$$

where α_1, α_2, and α_3 are the normalized rates with respect to biomass X. These are the specific kinetic rates. Thus, the mathematical model of the process is written in the following matrix form:

$$\begin{pmatrix} \dot{X} \\ \dot{S} \\ \dot{P} \end{pmatrix} = X \begin{pmatrix} \alpha_1 \\ -\alpha_2 \\ \alpha_3 \end{pmatrix}. \tag{20}$$

It is easy to see that the system in Eq. 20 is in the form of Eq. 8, with

$$\xi' = \xi \overset{\Delta}{=} \begin{pmatrix} X \\ S \\ P \end{pmatrix}; \qquad K' = K \overset{\Delta}{=} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

$$H \overset{\Delta}{=} \begin{pmatrix} X & 0 & 0 \\ 0 & X & 0 \\ 0 & 0 & X \end{pmatrix}; \qquad \alpha \overset{\Delta}{=} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} \qquad \text{and} \qquad W \overset{\Delta}{=} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Thus, the parameters, α_1, α_2, and α_3 can be estimated using an estimator of the form of Eq. 17 (for the continuous-time version) and Eq. 18 (for the discrete-time version). Since the measurements of X, S, and P are only available at sampling times, we will use the discrete-time estimator and we will discuss in particular and illustrate the choice of the tuning parameter θ. The discrete version of the estimator is

$$\begin{cases} \hat{X}_{t+1} = \hat{X}_t + T_s\left[\hat{\alpha}_{1t} X_t - 2\theta\left(\hat{X}_t - X_t\right)\right] \\ \hat{S}_{t+1} = \hat{S}_t - T_s\left[\hat{\alpha}_{2t} X_t - 2\theta\left(\hat{S}_t - S_t\right)\right] \\ \hat{P}_{t+1} = \hat{P}_t + T_s\left[\hat{\alpha}_{3t} X_t - 2\theta\left(\hat{P}_t - P_t\right)\right] \\ \hat{\alpha}_{1(t+1)} = \hat{\alpha}_{1t} - \dfrac{T_s\theta^2}{X_t}\left(\hat{X}_t - X_t\right) \\ \hat{\alpha}_{2(t+1)} = \hat{\alpha}_{2t} + \dfrac{T_s\theta^2}{X_t}\left(\hat{S}_t - S_t\right) \\ \hat{\alpha}_{3(t+1)} = \hat{\alpha}_{3t} - \dfrac{T_s\theta^2}{X_t}\left(\hat{P}_t - P_t\right). \end{cases} \tag{21}$$

In fact, the requirement that θ's value be chosen in practical situations is quite mild: it is the value that gives rise to the best estimates $\hat{X}$, $\hat{S}$, and $\hat{P}$ of the measured states X, S, and P. In other words, the validation procedure for choosing θ is based on a comparison between estimates of X, S, and P obtained via the estimated reaction rates α_1, α_2, and α_3 and the true measured values of X, S, and P. In order to illustrate this point, we have implemented three versions of estimator, Eq. 21, which only differs in the value of θ, which was equal to 0.5, 1, and 1.9, respectively. We notice that the sampling times are approximately equally spaced with $T_s \simeq 0.5$ h. As a result, θ has to be chosen such that $\theta T_S < 2$. In Figure 1, each real measurement X, S, and P is compared with the corresponding estimate obtained with $\theta = 0.5$, $\theta = 1$, and $\theta = 1.9$. This figure clearly shows that $\theta = 1$ constitutes a good compromise between a good tracking of the parameters' variations and a satisfactory noise rejection. Indeed, $\theta = 1.9$ provides somewhat accurate but noisy estimates, while $\theta = 0.5$ leads to smoothed but inaccurate ones. The estimated kinetic rates α_1, α_2, and α_3 obtained with the three values of θ are reproduced in Figure 2. They confirm the preceding remarks: the curves corresponding to $\theta = 1.9$ are very noisy, while those obtained with $\theta = 0.5$ do not vary enough to track the rapid variations of the kinetic rates.

Estimation of an Esterification Reaction Rate in a Reaction Calorimeter

The reaction being considered is an esterification held in a solvent and a highly alkaline medium. For reasons of confidentiality, we cannot give further details of the reaction itself. It takes place in a fed-batch jacketed reaction calorimeter that has been designed and tested in our laboratory (Fiaty, 1991; Crouslé, 1996). The acid is continuously added to the calorimeter containing the alcohol, with a dilution rate D and an input temperature $T_{R_{in}}$. Since only one reaction is considered, estimation of the corresponding rate can be achieved solely from the temperature measurements. As a result, the model we considered for the estimator design only accounts for the dynamics of the reactor temperature, and is written as follows:

$$\dot{T}_R = -\frac{q_r}{C_R} + \frac{UA}{C_R}\left(T_j - T_R\right) + D\left(T_{Rin} - T_R\right), \qquad (22)$$

where q_r is the reaction heat release and the other terms have the same meaning as before. It is well known that the term q_r is related to the reaction rate r through the following equation:

$$r = -\frac{q_r}{\Delta H V_R}. \qquad (23)$$

Estimation of q_r does not necessitate knowing the reaction enthalpy ΔH. Moreover, the latter can be estimated as follows:

$$\Delta H = \frac{\int_{t_1}^{t_2} q_r(t)\, dt}{n_2 - n_1}, \qquad (24)$$

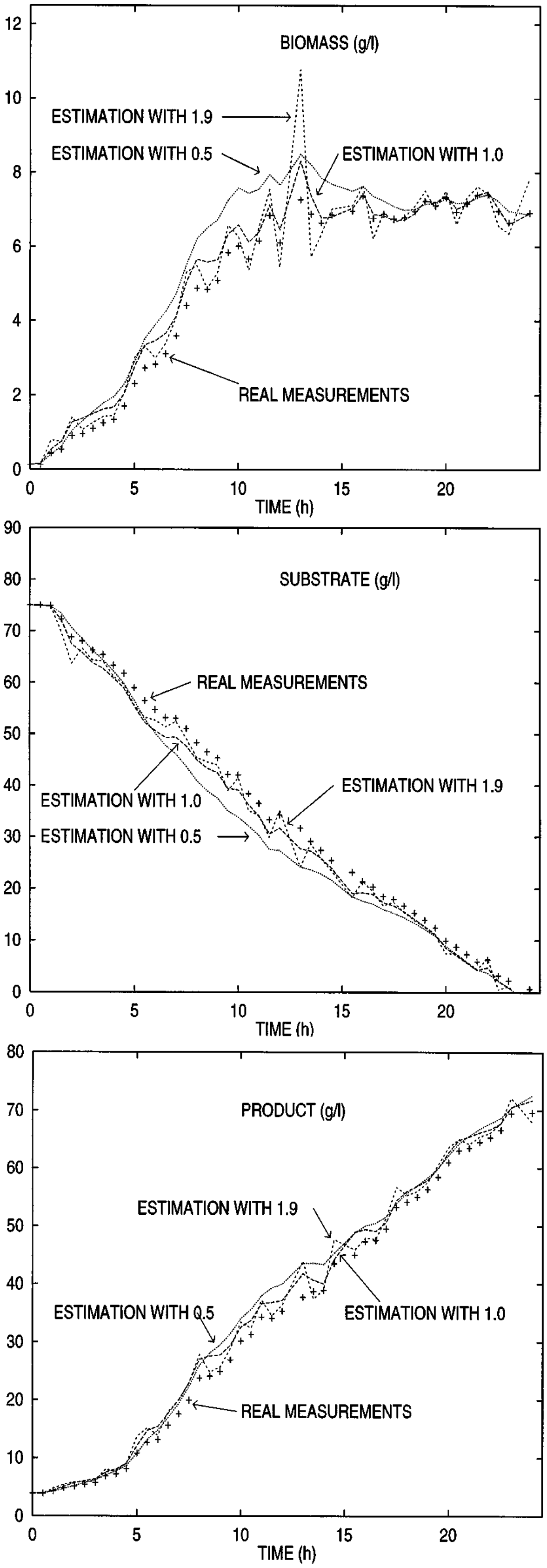

Figure 1. Comparison of *X*, *S*, and *P* estimates, obtained through three values of θ, with the real data measurements.

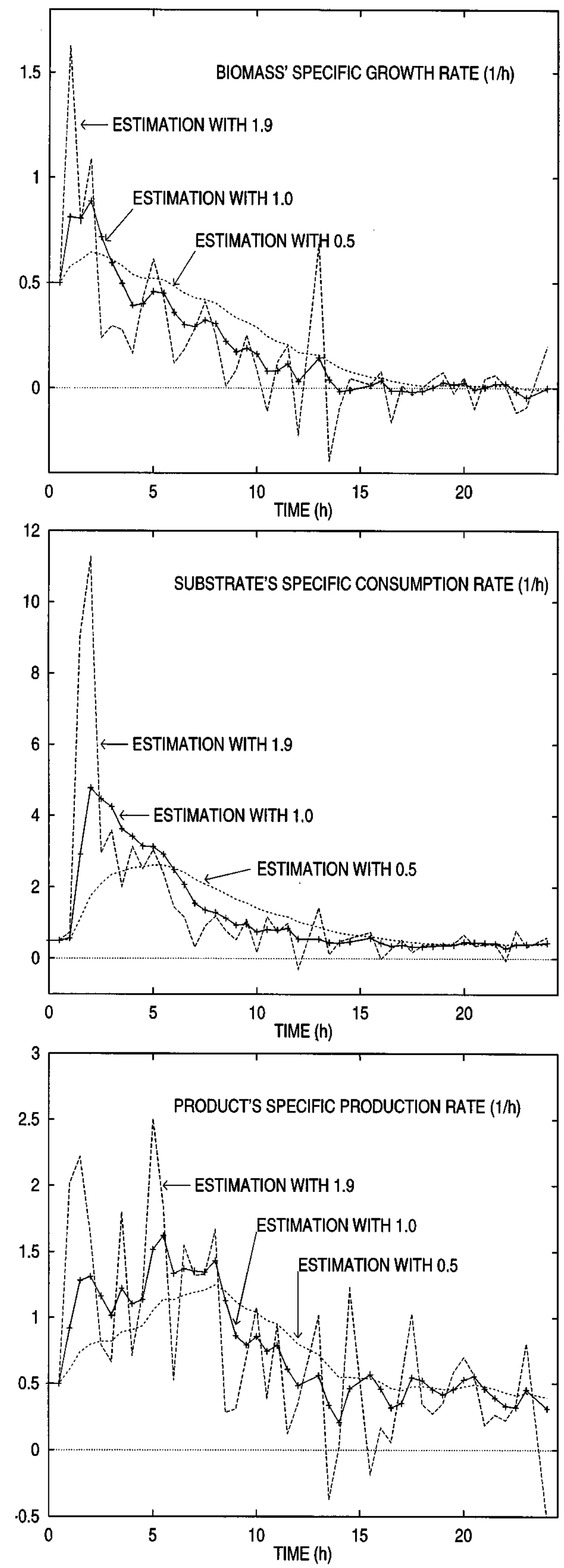

Figure 2. Comparison of three on-line estimates of the reaction rates obtained through three values of θ.

where t_1 and t_2 denote, respectively, the beginning and ending times of the reaction, and n_1 and n_2 denote the alcohol mole number at t_1 and t_2, respectively.

The equations of the discrete nonlinear observer used for the estimation of q_r are

$$\begin{cases} \hat{T}_{Rt+1} + \hat{T}_{Rt} + T_s\Big[-\dfrac{\hat{q}_{rt}}{C_R} + \dfrac{UA}{C_R}\left(T_{jt} - T_{Rt}\right) \\ \qquad\qquad + D(T_{Rin} - T_{Rt}) - 2\theta\left(\hat{T}_{Rt} - T_{Rt}\right)\Big] \\ \hat{q}_{rt+1} = \hat{q}_{rt} + T_s\theta^2 C_R\left(\hat{T}_{Rt} - T_{Rt}\right). \end{cases} \tag{25}$$

In order to get an initial idea of the value of θ to be used, we have reconstructed the time evolution of a square-wave electrical power signal, UI, that took place in the reactor before the reaction began. This estimation was provided by estimator, Eq. 25, where q_r was replaced by UI and $D = 0$. The temperatures T_R and T_j were available every 2 s, and the terms UA and C_R were assumed to be constant. Similarly, in order to gain confidence in the q_r estimate and the values of C_R and UA used, after the reaction we again estimated the square wave electrical power signal, UI, that occurred in the reactor. The θ value used by all estimators was equal to 0.05, and the values of the different parameters appearing in the model are

$$D = 0.00038\ \mathrm{h}^{-1} \qquad C_R = 1{,}600\ \mathrm{J \cdot K}^{-1}$$

$$UA = 4.4\ \mathrm{W \cdot K}^{-1} \qquad T_{Rin} = 295\ \mathrm{K}.$$

The progression of T_R and T_j along the reaction, plus the estimation of the reaction heat release, are given in Figure 3. Figure 4 shows the postreaction comparison between the electrical power signal and its estimate, as provided by the estimator, Eq. 25. We note how well the estimator reconstructed the electrical signal.

In order to check the consistency of the estimate of q_r, we used it to estimate the alcohol concentration inside the reactor. Indeed, letting C_A be the alcohol concentration, we have

$$\dot{C}_A = -r - DC_A = \frac{q_r}{\Delta HV_R} - DC_A. \tag{26}$$

Now, let us consider the following dynamical system:

$$\dot{\hat{C}}_A = \frac{\hat{q}_r}{\Delta HV_R} - D\hat{C}_A, \tag{27}$$

where $\hat{q}_r$ is the estimate of q_r provided by estimator, Eq. 25. Now, we can easily show that if the initial concentration of C_A is well known, then the numerical integration of Eq. 27 provides an estimate $\hat{C}_A$ of C_A that is as accurate as the estimate $\hat{q}_r$ of q_r. Such a result is also valid in the discrete case (by considering the forward Euler discretization). Indeed, we have solved the discrete version of Eq. 27 and we have compared the time evolution of $\hat{C}_A$, that is, the alcohol concen-

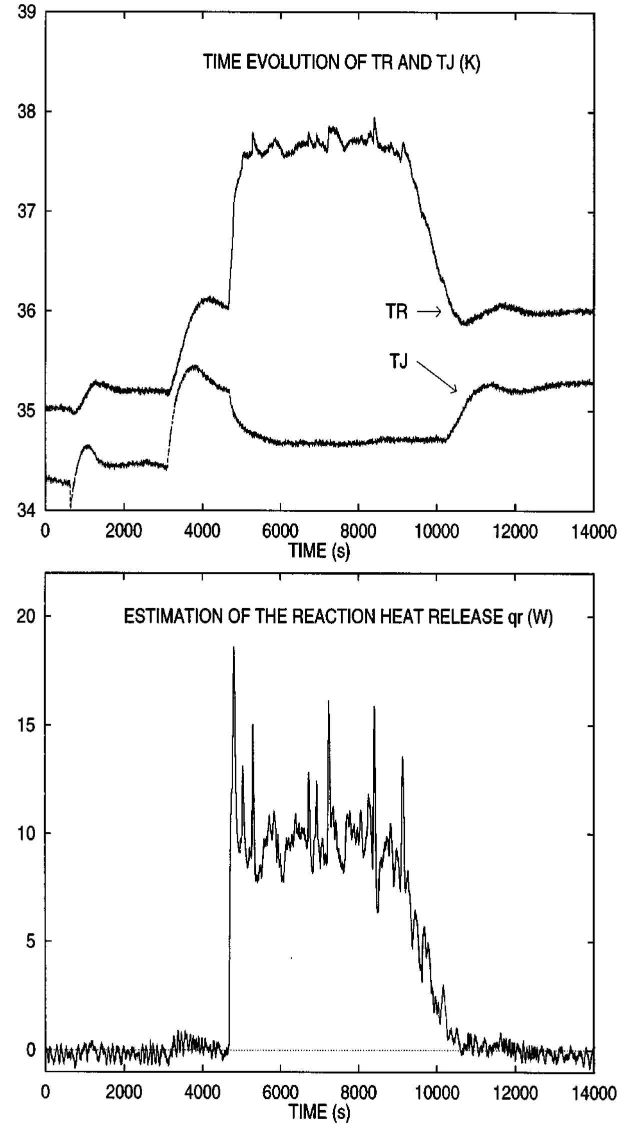

Figure 3. Estimation of the reaction heat release q_r using T_R and T_j measurements.

tration estimate, with off-line data. Corresponding results are reported in Figure 5. We note that the curve of the estimated concentration fits very well the available measurements. Such results confirm the usefulness of the proposed estimators in practical situations.

Conclusion

We have derived simple nonlinear observer-based estimators that allow on-line estimation of the reaction rates inside chemical and biochemical reactors. These estimators, whose convergences have been established in the continuous and discrete cases, are directly synthesized from the dynamical balance model of the processes. Their implementation, and their calibration in particular, is simple and easy to carry out; it is achieved through the tuning of a single parameter, whatever the number of components and reactions being considered. Experimental results were given, and they demonstrated how well the given estimators coped with nonlinearities and parameter uncertainties in chemical and biochemical systems.

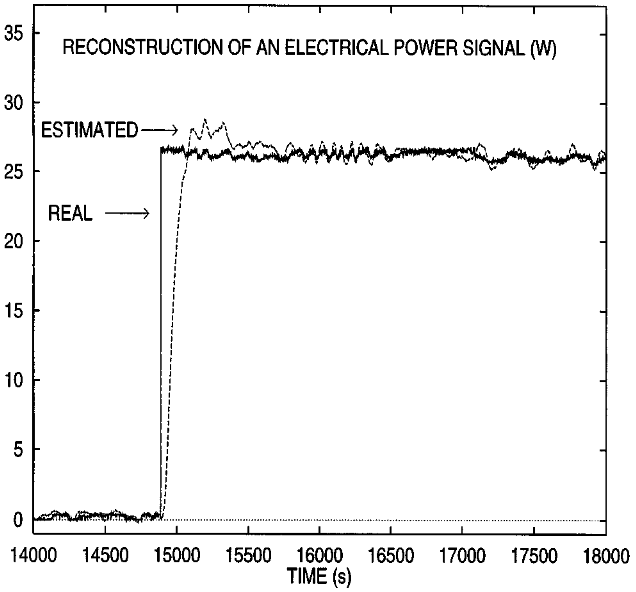

Figure 4. Estimation of an electrical power signal after the reaction.

However, some points may be raised by the proposed estimators. One of these concerns the fact that the estimator design assumes that the measurements of some component concentrations are available on-line. In some instances, such assumption may not be borne out in practice. For example, the measurement of biomass concentration in a fermentor is

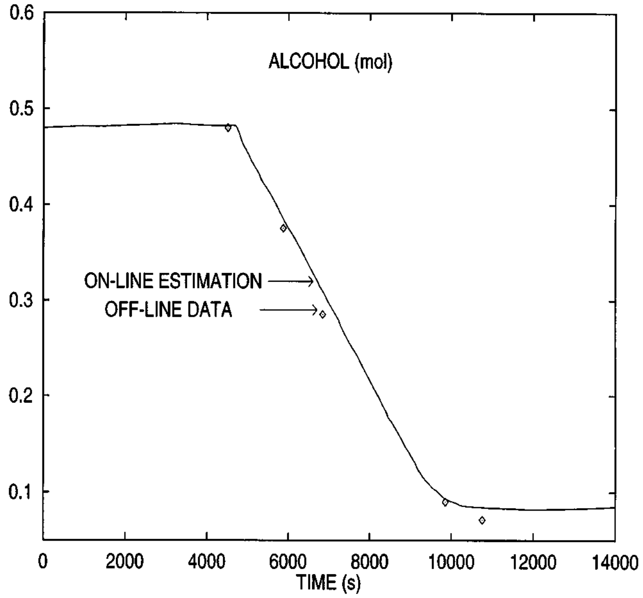

Figure 5. Comparison of the alcohol mole-number estimation with off-line data.

usually done manually through batchwise analysis, and generally takes an unreasonable amount of time to complete. Another consideration concerns the estimation of the reaction rates in chemical reactors. We have supposed throughout this article that some terms, such as UA or C_R, are known or constant. In some instances, however, these terms may vary along the reaction and need to be estimated. For the sake of clarity, these points are not treated in this article, but will be discussed elsewhere.

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Appendix A

Proof of Theorem 1. A simple computation shows that

$$S_\theta = \frac{1}{\theta}\Delta_\theta S_1 \Delta_\theta$$

where

$$S_1 = S_{\theta \mid \theta = 1} \qquad \text{and} \qquad \Delta_\theta = \begin{bmatrix} I_n & 0 \\ 0 & \dfrac{1}{\theta} I_n \end{bmatrix}.$$

Now, using Assumption A1, $\Lambda(\hat{z}_1, s)$ is invertible and the following equalities can easily be established: $F(\hat{z}_1, s) = \Lambda^{-1}(\hat{z}_1, s) A \Lambda(\hat{z}_1, s)$ and $C\Lambda(\hat{z}_1, s) = C$.

Thus, by multiplying the left and the right side of Eq. 16 by $\Lambda^T(\hat{z}_1, s)$ and $\Lambda(\hat{z}_1, s)$, respectively, we obtain

$$\theta \bar{S}_\theta(\hat{z}_1, s) + F^T(\hat{z}_1, s)\bar{S}_\theta(\hat{z}_1, s) + \bar{S}_\theta(\hat{z}_1, s) F(\hat{z}_1, s) - C^T C = 0, \quad \text{(A1)}$$

where $\bar{S}_\theta(\hat{z}_1, s) = \Lambda^T(\hat{z}_1, s) S_\theta \Lambda(\hat{z}_1, s)$.

Set $e(t) = \hat{z}(t) - z(t)$; then

$$\dot{e} = \left(F(\hat{z}_1, s) - \Lambda^{-1}(\hat{z}_1, s) S_\theta^{-1} C^T C\right) e + F(\hat{z}_1, s) z - (z_1, s) z + B(u, \hat{z}_1, s) - B(u, z_1, s) - \bar{\epsilon}(t).$$

Now, set $\bar{e} = \Delta_\theta \Lambda(\hat{z}_1, s) e$. We then obtain:

$$\begin{aligned}\dot{\bar{e}} = {} & \theta\left(A - S_1^{-1} C^T C\right)\bar{e} + \dot{\Lambda}(\hat{z}_1, s)\Lambda^{-1}(\hat{z}_1, s)\bar{e} \\ & + \Delta_\theta \Lambda(\hat{z}_1, s)\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right) \\ & + \Delta_\theta \Lambda(\hat{z}_1, s)\left(F(\hat{z}_1, s) z - F(z_1, s) z\right) + \Delta_\theta \Lambda(\hat{z}_1, s)\bar{\epsilon}(t).\end{aligned}$$

The last equality comes from the preceding remarks and from the fact that Δ_θ and Δ_θ^{-1} commute with each of the following matrices: $\Lambda(\hat{z}_1, s)$, $\Lambda^{-1}(\hat{z}_1, s)$, and $\dot{\Lambda}(\hat{z}_1, s)$.

Consider the quadratic function $V(\bar{e}) = \bar{e}^T S_1 \bar{e}$; then

$$\begin{aligned}
\dot{V} &= 2\bar{e}^T S_1 \dot{\bar{e}} \\
&= \theta\left(2\bar{e}^T S_1 A\bar{e} - 2\bar{e}^T C^T C\bar{e}\right) + 2\bar{e}^T S_1 \dot{\Lambda}(\hat{z}_1, s)\Lambda^{-1}(\hat{z}_1, s)\bar{e} \\
&\quad + 2\bar{e}^T S_1 \Delta_\theta \Lambda(\hat{z}_1, s)\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right) \\
&\quad + 2\bar{e}^T S_1 \Delta_\theta \Lambda(\hat{z}_1, s)\left(F(\hat{z}_1, s)z - F(z_1, s)z\right) \\
&\quad - 2\bar{e}^T S_1 \Delta_\theta \Lambda(\hat{z}_1, s)\bar{\boldsymbol{\epsilon}}(t) \\
&= -\theta V - \theta\|C\bar{e}\|^2 + 2\bar{e}^T S_1 \dot{\Lambda}(\hat{z}_1, s)\Lambda^{-1} \\
&\quad \times(\hat{z}_1, s)\bar{e} + 2\bar{\boldsymbol{\epsilon}}^T S_1 \Delta_\theta A\Lambda(\hat{z}_1, s)\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right) \\
&\quad + 2\bar{e}^T S_1 \Delta_\theta \Lambda(\hat{z}_1, s)\left(F(\hat{z}_1, s)z - F(z_1, s)z\right) \\
&\quad - 2\bar{e}^T S_1 \Delta_\theta \Lambda(\hat{z}_1, s)\bar{\boldsymbol{\epsilon}}(t)
\end{aligned}$$

by Eq. 12.

Therefore,

$$\begin{aligned}
\dot{V} &\leq -\theta V + 2\|S_1\bar{e}\|\,\|\dot{\Lambda}(\hat{z}_1, s)\Lambda^{-1}(\hat{z}_1, s)\|\,\|\bar{e}\| \\
&\quad + 2\|S_1\bar{e}\|\,\|\Lambda(\hat{z}_1, s)\|\,\|\Delta_\theta\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right)\| \\
&\quad + 2\|S_1\bar{e}\|\,\|\Delta_\theta\Lambda(\hat{z}_1, s)\left(F(\hat{z}_1, s)z - F(z_1, s)z\right)\| \\
&\quad + \frac{2}{\theta}\|S_1\bar{e}\|\,\|F_1(\hat{z}_1, s)\boldsymbol{\epsilon}(t)\| \leq -\theta V + 2k\|S_1\bar{e}\|\,\|\bar{e}\| \\
&\quad + 2\gamma\|S_1\bar{e}\|\,\|\Delta_\theta\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right)\| \\
&\quad + 2\|S_1\bar{e}\|\,\|\Delta_\theta\Lambda(\hat{z}_1, s)\left(F(\hat{z}_1, s)z - F(z_1, s)z\right)\| \\
&\quad + \frac{2\delta\beta}{\theta}\|S_1\bar{e}\|,
\end{aligned}$$

where $k = \sup_{t \geq 0} \|\dot{\Lambda}(\hat{z}_1, s)\Lambda^{-1}(z_1, s)\|$; δ is the upper bound of $\|\boldsymbol{\epsilon}(t)\|$; γ is the upper bound of $\|\Lambda(\hat{z}_1, s)\|$; and β is given in Assumption A1.

On the other hand, we have:

$$\begin{aligned}
\|\Delta_\theta\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right)\| &\leq \|b_1(u, \hat{z}_1, s) \\
&\quad - b_1(u, z_1, s)\| + \left\|\frac{1}{\theta}\left(b_2(u, \hat{z}_1, s) - b_2(u, z, s)\right)\right\| \\
&\leq \rho_1\|e_1\| + \frac{\rho_2}{\theta}\|e_1\|,
\end{aligned}$$

where ρ_1, ρ_2 denote the Lipschitz constants of b_1 and b_2, respectively.

Now, assuming that $\theta > \theta' = \min\{1, \rho_2\}$, we obtain:

$$\begin{aligned}
\|\Delta_\theta\left(B(u, \hat{z}_1, s) - B(u, z_1, s)\right)\| &\leq \rho_1\|e_1\| \\
&\quad + \rho_2'\|e_1\| \leq \rho\|\bar{e}\|,
\end{aligned}$$

where $\rho = \rho_1 + \rho_2'$, $\rho_2' = \rho_2$ if $\rho_2 > 1$, and $\rho_2' = 1$ otherwise.

Similarly,

$$\begin{aligned}
\|\Delta_\theta\Lambda(\hat{z}_1, s)\left(F(\hat{z}_1, s)z - F(z_1, s)z\right)\| &= \|F_1(\hat{z}_1, s)z_2 \\
&\quad - F_1(z_1, s)z_2\| \leq \zeta\|e_1\| \leq \zeta\|\bar{e}\|
\end{aligned}$$

for some positive constant ζ depending on the upper bound of s and z_2.

Hence,

$$\dot{V} \leq -\theta V + c_1 V + \frac{c_2}{\theta}\sqrt{V} \tag{A2}$$

where $c_1 = (2k + 2\gamma\rho + 2\zeta)\sigma(S_1)$ and $c_2 = 2\delta\beta\sqrt{\lambda_{\max}(S_1)}$ with

$$\sigma(S_1) = \sqrt{\frac{\lambda_{\max}(S_1)}{\lambda_{\min}(S_1)}};$$

$\lambda_{\max}(S_1)$ [resp., $\lambda_{\min}(S_1)$] is the largest [resp., the smallest] eigenvalue of S_1.

Thus,

$$\frac{d}{dt}\left(\sqrt{V(\bar{e}(t))}\right) \leq -\frac{(\theta - c_1)}{2}\sqrt{V(\bar{e}(t))} + \frac{c_2}{2\theta}.$$

Consequently,

$$\begin{aligned}
\sqrt{V(\bar{e}(t))} &\leq \exp\left[-\left(\frac{\theta - c_1}{2}\right)t\right]\sqrt{V(\bar{e}(0))} \\
&\quad + \frac{c_2}{\theta(\theta - c_1)}\left[1 - \exp\left[-\left(\frac{\theta - c_1}{2}\right)t\right]\right].
\end{aligned}$$

Now taking $\theta_0 = \max\{\theta', c_1\}$ and $\theta > \theta_0$, we obtain

$$\begin{aligned}
\|\bar{e}(t)\| &\leq \sigma(S_1)\exp\left[-\left(\frac{\theta - c_1}{2}\right)t\right]\|\bar{e}(0)\| \\
&\quad + \frac{c_2}{\theta(\theta - c_1)\sqrt{\lambda_{\min}(S_1)}}.
\end{aligned} \tag{A3}$$

On the other hand, we have:

$$\kappa_\theta\|e(t)\|^2 \leq \|\bar{e}(t)\|^2 \leq \breve{\kappa}_\theta\|e(t)\|^2, \tag{A4}$$

where $\kappa_\theta = \min\{1, (\alpha^2/\theta^2)\}$ and $\breve{\kappa}_\theta = \max\{1, (\beta^2/\theta^2)\}$; α and β are given in Assumption A1.

Combining Eqs. A1 and A2, and replacing c_2 by the preceding expression, we obtain

$$\begin{aligned}
\|e(t)\| &\leq \sigma(S_1)\sqrt{\frac{\breve{\kappa}_\theta}{\kappa_\theta}}\exp\left[-\left(\frac{\theta - c_1}{2}\right)t\right]\|e(0)\| \\
&\quad + \frac{2\sigma(S_1)\beta}{\theta(\theta - c_1)\sqrt{\kappa_\theta}}\delta.
\end{aligned}$$

Now, it is easy to see that θ_0, λ_θ, μ_θ, and M_θ needed by Theorem 1 are

$$\theta_0=\max\{\min\{1,\rho_2\},c_1\},\qquad \lambda_\theta=\sigma(S_1)\sqrt{\frac{\breve{\kappa}_\theta}{\kappa_\theta}},$$

$$\mu_\theta=\frac{\theta-c_1}{2},\qquad \text{and}\qquad M_\theta=\frac{2\sigma(S_1)\beta}{\theta(\theta-c_1)\sqrt{\kappa_\theta}}.$$

This ends the proof of Theorem 1.

Appendix B

Proof of theorem 2

The proof of Theorem 2 is based on the following claim:

Claim 1. Set $\tilde{A}_t=[I_{2n}+\theta T_s(A-S_1^{-1}C^TC)]$ where

(i) $A=\begin{bmatrix}0 & I_n\\ 0 & 0\end{bmatrix}$,

(ii) S_1 is given by Eq. 12 for $\theta=1$,

(iii) I_{2n} is the $2n\times 2n$ identity matrix.

Then, for all $T_s>0$ and $\theta>0$ such that $\theta\ T_s<1$, the unique symmetric positive definite matrix P satisfying the algebraic equation

$$\tilde{A}^TP\tilde{A}-P=-\theta T_sP-\theta T_s(1-\theta T_s)^2C^TC \tag{B1}$$

is given by

$$P=\begin{bmatrix}I_n & -I_n\\ -I_n & (2-\theta T_s)I_n\end{bmatrix}.$$

This claim can be proved by simple verification.

Proof of Theorem 2. Setting $e_t=\hat{z}_t-z_t$, then

$$e_{t+1}=\left[I_{2n}+T_s\left(F(y_t,s_t)-\Lambda^{-1}(y_t,s_t)S_\theta^{-1}C^TC\right)\right]e_t-T_s\bar{\epsilon}_t.$$

Hereafter, we shall denote any matrix $Q(y_t,s_t)$ by Q_t (for example, $\Lambda(y_t,s_t)=\Lambda_t$, $F_{1(t+1)}=F_1(y_{t+1},s_{t+1})$, etc.).

Set $\bar{e}_t=\Lambda_t\Delta_\theta e_t$. Then, routine computations give

$$\begin{aligned}\bar{e}_{t+1}&=\Lambda_{t+1}\Lambda_t^{-1}\tilde{A}\bar{e}_t-T_s\Lambda_{t+1}\Delta_\theta\bar{\epsilon}_t\\ &=\tilde{A}\bar{e}_t+\left(\Lambda_{t+1}\Lambda_t^{-1}-I_{2n}\right)\tilde{A}\bar{e}_t-T_s\Lambda_{t+1}\Delta_\theta\bar{\epsilon}_t,\end{aligned} \tag{B2}$$

where $\tilde{A}$ is as in Claim 1.

Consider the time-varying quadratic function $V_t=\sqrt{\bar{e}_t^TP\bar{e}_t}=\|N\bar{e}_t\|$, where

$$N=\begin{bmatrix}I_n & -I_n\\ 0 & \sqrt{1-\theta T_s}\,I_n\end{bmatrix}$$

is obtained by the Cholesky decomposition $P=N^TN$. Moreover, one can easily check that

$$N=\Gamma U$$

where

$$\Gamma=\begin{bmatrix}I_n & 0\\ 0 & \sqrt{1-\theta T_s}\,I_n\end{bmatrix}\qquad\text{and}\qquad U=\begin{bmatrix}I_n & -I_n\\ 0 & I_n\end{bmatrix}.$$

In fact, the matrix U satisfies $S_1=U^TU$, where $S_1=S_{|\theta=1}$. According to this, we have

$$\lambda_{\min}(P)\geq\frac{\lambda_{\min}(S_1)}{1-\theta T_s}\qquad\text{and}\qquad\lambda_{\max}(P)\leq\lambda_{\max}(S_1), \tag{B3}$$

where $\lambda_{\min}(\cdot)$ and $\lambda_{\max}(\cdot)$ stand for the largest and smallest eigenvalue, respectively.

Now, we have

$$\begin{aligned}V_{t+1}&=\|N\bar{e}_{t+1}\|\leq\|N\tilde{A}\bar{e}_t\|+\|N\left(\Lambda_{t+1}\Lambda_t^{-1}-I_{2n}\right)\tilde{A}\bar{e}_t\|\\ &\quad+T_s\|N\Lambda_{t+1}\Delta_\theta\bar{\epsilon}_t\|\leq\|N\tilde{A}\bar{e}_t\|\\ &\quad+\|N\left(\Lambda_{t+1}\Lambda_t^{-1}-I_{2n}\right)N^{-1}\|\,\|N\tilde{A}\bar{e}_t\|+T_s\|N\Lambda_{t+1}\Delta_\theta\bar{\epsilon}_t\|.\end{aligned}$$

By Claim 1, we have

$$\begin{aligned}\|N\tilde{A}\bar{e}_t\|^2&=\bar{e}_t^T\tilde{A}^TN^TN\tilde{A}\bar{e}_t=\bar{e}_t^T\tilde{A}^TP\tilde{A}\bar{e}_t=(1-\theta T_s)\bar{e}_t^TP\bar{e}_t\\ &\quad-\theta T_s(1-\theta T_s)^2\bar{e}_t^TC^TC\bar{e}_t\leq(1-\theta T_s)\|N\bar{e}_t\|^2.\end{aligned}$$

Hence $\|N\tilde{A}\bar{e}_t\|\leq\sqrt{1-\theta T_s}\,\|N\bar{e}_t\|=\sqrt{1-\theta T_s}\,V_t$.

Using the last inequality, we get

$$\begin{aligned}V_{t+1}&\leq\sqrt{(1-\theta T_s)}\left(1+\|N\left(\Lambda_{t+1}\Lambda_t^{-1}-I_{2n}\right)N^{-1}\|\right)V_t\\ &\quad+T_s\|N\Lambda_{t+1}\Delta_\theta\bar{\epsilon}_t\|.\end{aligned} \tag{B4}$$

A simple computation gives

$$\begin{aligned}&N\left(\Lambda_{t+1}\Lambda_t^{-1}-I_{2n}\right)N^{-1}\\ &=\begin{bmatrix}\left(I_n-F_{1(t+1)}F_{1t}^{-1}\right) & 0\\ 0 & \left(I_n-F_{1(t+1)}F_{1t}^{-1}\right)\end{bmatrix}\begin{bmatrix}0 & \dfrac{1}{\sqrt{1-\theta T_s}}\\ 0 & -1\end{bmatrix}.\end{aligned}$$

Hence

$$\begin{aligned}\|N\left(\Lambda_{t+1}\Lambda_t^{-1}-I_{2n}\right)N^{-1}\|&\leq\|I_n-F_{1(t+1)}F_{1t}^{-1}\|\sqrt{\frac{2-\theta T_s}{1-\theta T_s}}\\ &\leq\eta\sqrt{\frac{2-\theta T_s}{1-\theta T_s}},\end{aligned} \tag{B5}$$

where η is given in Assumption A6.

On the other hand, we have

$$\|N\Lambda_{t+1}\Delta_\theta\bar{\epsilon}_t\|\leq\frac{\beta\sqrt{2-\theta T_s}}{\theta}\delta, \tag{B6}$$

where β is given is Assumption A1 and δ denotes the upper bound of $\|\epsilon\|$.

Combining Eqs. B4, B5, and B6,

$$V_{t+1} \leq \sqrt{1-\theta T_s}\left(1+\eta\sqrt{\frac{2-\theta T_s}{1-\theta T_s}}\right)V_t + \frac{T_s\beta\sqrt{2-\theta T_s}}{\theta}\delta$$

$$= \left(\sqrt{1-\theta T_s}+\eta\sqrt{2-\theta T_s}\right)V_t + \frac{T_s\beta\sqrt{2-\theta T_s}}{\theta}\delta$$

$$\leq \left(\sqrt{1-\theta T_s}+\eta\left(1+\sqrt{1-\theta T_s}\right)\right)V_t + \frac{T_s\beta\sqrt{2-\theta T_s}}{\theta}\delta$$

$$= \left(\eta+(1+\eta)\sqrt{1-\theta T_s}\right)V_t + \frac{T_s\beta\sqrt{2-\theta T_s}}{\theta}\delta. \qquad \text{(B7)}$$

Now, for a given T_s satisfying Assumption A6, choose θ such that

$$\theta_0 = \frac{1}{T_s}\left(1-\left[\frac{1-\eta}{1+\eta}\right]^2\right) < \theta < \frac{1}{T_s} = \theta_1. \qquad \text{(B8)}$$

It follows that

$$d_\theta = \eta + (1+\eta)\sqrt{1-\theta T_s} < 1.$$

The discrete inequality Eq. B7 gives rise to

$$V_t \leq (d_\theta)^t V_0 + \left(\sum_{i=0}^{t-1}(d_\theta)^{t-1-i}\right)\frac{T_s\beta\sqrt{2-\theta T_s}}{\theta}\delta$$

$$\leq (d_\theta)^t V_0 + \left(\frac{1-(d_\theta)^t}{1-d_\theta}\right)\frac{T_s\beta\delta}{\theta}\sqrt{1+\left(\frac{1-\eta}{1+\eta}\right)^2}.$$

Hence,

$$\|\bar{e}_t\| \leq \sigma(P)(d_\theta)^t\|\bar{e}_0\| + \left(\frac{1-(d\theta)^t}{1-d_\theta}\right)\frac{T_s\beta\delta}{\theta\sqrt{\lambda_{\min}(P)}}\sqrt{1+\left(\frac{1-\eta}{1+\eta}\right)^2},$$

with $\sigma(\cdot) = \sqrt{\lambda_{\max}(\cdot)/\lambda_{\min}(\cdot)}$.

Using inequalities B3, simple computations give rise to

$$\|\bar{e}_t\| \leq \overline{m}_{1\theta}(d_\theta)^t\|\bar{e}_0\| + \overline{m}_{2\theta}\delta$$

for some constants $\overline{m}_{1\theta} > 0$ and $\overline{m}_{2\theta} > 0$.

Finally, using Inequality A4, we obtain

$$\|e_t\| \leq m_{1\theta}(d_\theta)^t\|e_0\| - m_{2\theta}\delta$$

for some constants $m_{1\theta} > 0$ and $m_{2\theta} > 0$.

This ends the proof of Theorem 2.

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