State Observers for Reaction Systems with Improved Convergence Rates

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Abstract

The problem of designing state observers for reaction systems whose convergence rate is faster than the standard asymptotic observers [7] is adressed in this paper. It is assumed that the reaction functions are known and that there are more measurements than "independent" reactions. If the unmeasurable state enters *linearly* in the reaction functions we propose an observer that converges in *finite-time*, under very weak excitation assumptions. If this dependence is *nonlinear*, we additionally assume that there is an element of the reaction functions vector that depends *only on one* unmeasurable state and that these functions are strictly monotonic. Under these conditions, a state observer that ensures *exponential convergence* of the states that appear in the reaction functions is designed. For the unmeasurable states that do not appear in these functions, the convergence is similar to the one of the asymptotic observers.

Keywords: Adaptive observer, Reaction system, Parameter estimation, Nonlinear systems

1. Introduction

A central question in process control is how to monitor reactant and product concentrations in a reliable and cost effective manner. In many

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practical applications, only some of the concentrations of the components are available for on-line measurement. A typical scenario is that dissolved oxygen concentration in bioreactors, temperature in non-isothermal reactors and gaseous flow rates are available for on-line measurement, but the values of the concentrations of products, reactants and/or biomass can only be determined via on-line analysis. The use of model-based state observers is a sensible way reconstruction these quantities using only a limited set of measurements—a topic that has attracted the attention of researchers in the process control and systems theory community for several years[1, 2, 5, 7, 8, 9, 10, 11, 12, 13, 14, 17, 19, 20, 21, 25, 27, 31, 32].

In this paper we are interested in the problem of state observation of reaction systems There are two important issues in this problem, first that the dynamics of these systems are highly nonlinear and uncertain, with the latter being typically associated with the imprecise knowledge of the reaction functions parameters. Second, it has been known—for more than 30 years—that it is possible to exploit the particular structure of these systems to remove the need to know the uncertain reaction functions, designing the so-called "asymptotic observers" [7]. However, it is also well-known that the transient behavior of these kinetic-independent observers, being essentially an open-loop copy of the (transformed) system dynamics, may be practically inadmissible. In particular, a strong drawback is that there are no free parameters to "tune" their convergence rate, see [26, Remark 4].

In this paper, assuming knowledge of the reaction functions, we are interested in designing observers with *tunable and improved* convergence rates. Towards this end, we adopt a radically different approach to the problem. First, taking the perspective of the parameter estimation based observers (PEBOs) proposed in [28], the task of estimation of the states is translated into a *parameter* estimation problem. Second, when the reaction functions depend *linearly* in the unmeasurable state, the estimation of this parameter is carried out following the dynamic regressor extension and mixing (DREM) technique proposed in [3]. In this case, we propose an observer that converges in *finite-time*, under very weak sufficient excitation assumptions. If the dependence is *nonlinear*, we additionally assume that there is an element of the reaction functions vector that depends *only on one* unmeasurable state and that these functions are *strictly monotonic*. Under these conditions, we design an Immersion and Invariance (I&I) state observer [6, 23, 24] that, exploiting the aforementioned monotonicity property, ensures *exponential convergence* of the states that appear in the reaction functions. For the

unmeasurable states that do not appear in these functions, the convergence is the *same* as the one of the asymptotic observers.

Assuming knowledge of the reaction functions it is also possible to design high-gain observers [15, 16] that, as is well-known, exhibit a high sensitivity to noise that is unavoidable in reaction systems, see [4, 35] for recent illustrations of this fact.

The remainder of the paper is organized as follows. In Section 2 we formulate the observer problem studied in the paper and in Section 3 we briefly recall the construction of the asymptotic observers. Section 4 is devoted to the identification the class of systems considered in the paper. Section 5 presents a key lemma for the application of PEBO. Section 6 presents the main result for the case of linear dependence on the unmeasurable states of the reaction function, while the nonlinear case is treated in Section 7. In Section 8 we apply the results to three benchmark examples. In particular, we show that for the non-isothermal chemical stirred tank reactor it is possible to design an *adaptive* observer that does not requires the knowledge of the parameters of the reaction function. The paper is wrapped-up with conclusions and a discussion on future work in Section 9.

Notation For $m \in \mathbb{N}_+$ we define the set $\bar{m} := \{1, 2, \dots, m\}$. The error between a signal (or parameter) $(\cdot)$ and its estimate $\hat{(\cdot)}$ is denoted as $\tilde{(\cdot)} := \hat{(\cdot)} - (\cdot)$. For $x \in \mathbb{R}^n$ we denote $|x|^2 = x^\top x$ and $\mathrm{col}(x_i)$, $i \in \bar{n}$ denotes a column vector with elements x_i. All functions are assumed to be smooth. For a function of scalar argument we denote its derivative as $(\cdot)'$. To avoid the proliferation of constants we use the symbol κ to denote a *generic* positive constant. Also, we use the symbol $\xi_{(\cdot)}$ to denote *measurable* signals.

2. Problem Formulation

We consider reaction systems whose dynamical model is given by

$$\begin{aligned} \dot{c} &= -uc + Kr^0(c) + \xi \\ y &= Lc, \end{aligned} \tag{1}$$

with $c \in \mathbb{R}^n_+$ are the components concentrations, $r^0 : \mathbb{R}^n_+ \to \mathbb{R}^q_+$, with $q < n$, is the reaction rate vector, $K \in \mathbb{R}^{n \times q}$ is the constant stoichiometric coefficient matrix, $u \in \mathbb{R}_+$ is the dilution rate, and $\xi \in \mathbb{R}^n_+$ is the difference between the feedrate and the output flow. The full rank matrix $L \in \mathbb{R}^{m \times n}$, with

$m < n$, selects the measured components of c. It is assumed that u and ξ are *measurable* and K is *known* and we define

$$p := \text{rank } \{K\}, \tag{2}$$

where, clearly, $p \leq q$.

The elements of the reaction vector $r^0(c)$ are of the form[1]

$$r_k^0(c) = \prod_{i=1}^{n} r_{ki}^0(c_i), k \in \bar{q},$$

and

$$r_{ki}^0(c_i) \geq 0 \ , \ r_{ki}^0(0) = 0, \forall k \in \bar{q}, \forall i \in \bar{n}.$$

The model given above describes the behavior of a large class of chemical and bio-chemical reaction systems [7, 12].

To formulate the observation problem we partition the concentration vector c into its measurable and unmeasurable components $y \in \mathbb{R}^m$ and $x \in \mathbb{R}^d$, with $d := n - m$, as

$$\begin{bmatrix} y \\ x \end{bmatrix} = Wc, \ W := \begin{bmatrix} L \\ \star \end{bmatrix} \in \mathbb{R}^{n \times n}, \tag{3}$$

where W is *full-rank*, and we use $\star$ to denote non-relevant matrices of suitable dimensions. The problem is, then, to design an observer

$$\begin{aligned} \dot{\chi} &= F(y, u, \xi, \chi) \\ \hat{x} &= G(y, u, \xi, \chi), \end{aligned}$$

where $\chi \in \mathbb{R}^{n_\chi}$, that ensures $\lim_{t \to \infty} |\tilde{x}(t)| = 0$ with *improved* convergence properties, with respect to the classical asymptotic observers [7].

3. An Alternative Parameterization of the System (1)

The lemma below, which is the main result needed for the construction of the asymptotic observers, is instrumental for our development. Although

[1] If a particular element c_s, $s \in \bar{n}$, of the vector c does not appear in $r_k(c)$, we set the corresponding function r_{ks}^0 equal to one. A similar consideration is applied to all factorizations of $r_k^0(c)$ given below.

the proof may be found in [7, Subsection 3.3], to set-up the notation and for the sake of completeness, we give it also here.

To streamline the presentation of the lemma we impose, similarly to the requirement for the design of asymptotic observers, the following.

Assumption A1 There are *more* measurements than *linearly independent* reaction rates, that is,

$$m \geq p, \tag{4}$$

where p is defined in (2).

Lemma 1. Consider the system (1). There exists full rank matrices $P \in \mathbb{R}^{n\times n}$ and $Q \in \mathbb{R}^{q\times q}$, such that the following change of state coordinates and redefinition of the reaction rate vector

$$\begin{aligned} z = \begin{bmatrix} z_a \\ z_b \end{bmatrix} &:= Pc \\ r(z) = \begin{bmatrix} r_a(z) \\ r_b(z) \end{bmatrix} &:= Q^{-1} r^0(P^{-1}z) \end{aligned} \tag{5}$$

yields the dynamics

$$\begin{aligned} \dot{z}_a &= -uz_a + r_a(z) + \xi_a \\ \dot{z}_b &= -uz_b + \xi_b, \end{aligned} \tag{6}$$

where $z_a \in \mathbb{R}^p$, $r_a : \mathbb{R}^n \mapsto \mathbb{R}^p$ and the vector $\mathrm{col}(\xi_a, \xi_b)$ is *measurable*. Moreover, if Assumption A1 holds, there exists matrices $T_{z_b} \in \mathbb{R}^{d\times(n-p)}$ and $T_y \in \mathbb{R}^{d\times m}$ such that

$$x = T_{z_b} z_b + T_y y. \tag{7}$$

Proof. Invoking [22, Corollary 2.7.1] we have that there exist full-rank, square matrices P and Q such that

$$PKQ = \begin{bmatrix} I_p & 0_{p\times(q-p)} \\ 0_{(n-p)\times p} & 0_{(n-p)\times(q-p)} \end{bmatrix}. \tag{8}$$

From which we obtain (6).

Now, we have the following relations between the state vectors

$$z = \begin{bmatrix} z_a \\ z_b \end{bmatrix} = Pc = PW \begin{bmatrix} y \\ x \end{bmatrix} =: \begin{bmatrix} \star & \star \\ U_y & U_x \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix},$$

where we used (3) and, in an obvious way, defined the submatrices $U_y \in \mathbb{R}^{(n-p)\times m}$, $U_x \in \mathbb{R}^{(n-p)\times d}$. Under Assumption A1, U_x is a tall, full-rank matrix, consequently we can write

$$x = U_x^{\dagger}(z_b - U_y y),$$

where $U_x^{\dagger}$ is the Moore-Penrose pseudo-inverse of of U_x. The proof is completed defining

$$T_{z_b} := U_x^{\dagger},\ T_y := -U_x^{\dagger}U_y.$$

□□□

Equipped with Lemma 1 it is possible to design a reaction-independent observer as

$$\begin{aligned} \dot{\hat{z}}_b &= -u\hat{z}_b + \xi_b \\ \hat{x} &= T_{z_b}\hat{z}_b + T_y y. \end{aligned} \tag{9}$$

The error dynamics of the z_b coordinates clearly satisfies

$$\dot{\tilde{z}}_b = -u\tilde{z}_b,$$

whose solution is

$$\tilde{z}_b(t) = e^{-\int_0^t u(s)ds}\tilde{z}_b(0). \tag{10}$$

Hence, $\tilde{z}_b(t) \to 0$—and, consequently, $\tilde{x}(t) \to 0$—if and only if $u \notin \mathcal{L}_1$. The main problem of this observer is that it is not possible to "tune" the convergence rate, which is univocally defined by $u(t)$.

Remark 1. In some very particular cases, for instance the scenario considered in [26, Proposition 2], it is possible to tune the convergence rate under some strong observability conditions.[2]

4. Identification of the Class of Systems

In this section we state the assumptions needed to solve the observation problem posed in Section 2. To avoid the proliferation of symbols, and with some abuse of notation, we relabel the reaction rate sub-vector $r_a(z)$—defined in (5)—via the function $r_a : \mathbb{R}_+^m \times \mathbb{R}_+^d \to \mathbb{R}_+^p$, that is, $r_a(y,x) \leftarrow r_a(z)$ and denote its elements as $r_a(y,x) := \mathrm{col}(r_{a1}(y,x), \dots, r_{ap}(y,x))$.

We consider two different scenarios.

[2]The authors thank an anonymous reviewer for bringing this result to our attention.

S1 The reaction rate sub-vector $r_a(y, x)$ depends *linearly* on the unmeasurable components of the state x, that is, it is of the form

$$r_a(y, x) = R(y)x \tag{11}$$

where $R : \mathbb{R}^m \to \mathbb{R}^{p\times d}$.

S2 The dependence of $r_a(y, x)$ on x is *nonlinear*.

In the *nonlinear scenario* we additionally require the following.

Assumption A2 For the unmeasurable concentration x_ℓ, $\ell \in \bar{d}$, that we want to observe there exists an element of the reaction rates sub-vector, which depends *only* on this concentration. That is, for the given $\ell \in \bar{d}$, *there exists* an $k \in \bar{p}$, such that

$$r_{ak}(y, x_\ell) = r_{ak\ell}(x_\ell)\mu_{ak}(y), \tag{12}$$

where, for ease of future reference, we have defined the measurable signal

$$\mu_{ak}(y) := \prod_{j=1}^{m} r_{akj}(y_j),\ k \in \bar{p}.$$

Moreover, we assume that the functions $r_{ak\ell}(x_\ell)$ are, either, *strictly monotonically increasing* (SMI), that is,

$$(a - b)[r_{ak\ell}(a) - r_{ak\ell}(b)] \geq \kappa|a - b|^2,\ \forall a, b \in \mathbb{R}_+,\ a \neq b,$$

or *strictly monotonically decreasing* (SMD), *i.e.*,

$$(a - b)[r_{ak\ell}(a) - r_{ak\ell}(b)] \leq \kappa|a - b|^2,\ \forall a, b \in \mathbb{R}_+,\ a \neq b.$$

The following observations pertaining to the assumptions are in order.

O1 Assumption A1 is necessary for the design of asymptotic observers. It is satisfied if there are more measurement than reaction rates, that is, if $m \geq q$. As discussed in [26, Remark 4], the latter is necessary to ensure detectability of the state c when the reaction rates $r^0(c)$ are *unknown*.

O2 Examples of reaction functions that satisfy the SMI or SMD condition are linear $r_{ak\ell}(s) = \eta s$ and Arrhenius' $r_{ak\ell}(s) = e^{-\eta s}$ laws, with $\eta > 0$. The popular Monod's law, that is, $r_{ak\ell}(s) = \frac{s}{s+\eta}$, satisfies the assumption, but *without* the "strict" qualifier.[3] As will become clear below, in this case asymptotic, but not exponential, convergence of the observation error is still ensured.

O3 Assumption A2 ensures that there exists a reaction function where no products of unmeasurable states x_ℓ appear. This feature is necessary to be able to exploit the SMI or SMD property of these functions, when the latter depend nonlinearly in x. Although this assumption seems quite restrictive in some cases it is possible to recombine the equations of the measurable states to enforce it—see Subsubsection 8.3 for an example.

O4 To simplify the presentation, and without loss of generality, in the sequel we assume that all reaction functions are SMI. As will be shown below the difference between these two cases boils down to the selection of the sign of a free constant gain.

5. A Parameter Estimation-based Approach for Observer Design

In this section we show how, in the spirit of the PEBO proposed in [28], the task of estimation of the unmeasurable states x can be translated into a *parameter* estimation problem. The first step to carry out this task is to generate a linear regression equation for x. In the second step a new partial coordinate, whose dynamics is amenable for the application of parameter estimation techniques, is proposed.

5.1. Derivation of the linear regression

Lemma 2. Consider the dynamics of the partial coordinate z_b defined in (6) and the dynamic extension

$$\begin{aligned} \dot{\hat{z}}_b &= -u\hat{z}_b + \xi_b \\ \dot{w} &= -uw,\ w(0) = 1. \end{aligned} \tag{13}$$

Then, x given in (7) satisfies the *linear regression* equation

$$x = T_{z_b}\hat{z}_b + T_y y + w\theta, \tag{14}$$

[3] The authors thank an anonymous reviewer for pointing this to us.

where $\theta \in \mathbb{R}^d$ is an *unknown* constant vector.

Proof. From (10) and integration of the w equation in (13) we have that

$$\tilde{z}_b(t) = w(t)\tilde{z}_b(0).$$

Replacing the latter in (7) yields

$$\begin{aligned} x &= T_{z_b}(\hat{z}_b - \tilde{z}_b) + T_y y \\ &= T_{z_b}\hat{z}_b + T_y y - wT_{z_b}\tilde{z}_b(0) \end{aligned}$$

which coincides with (14) defining

$$\theta := T_{z_b}[z_b(0) - \hat{z}_b(0)].$$

□□□

Corollary 1. Consider (13) and (14) and define the observed state as

$$\hat{x} = T_{z_b}\hat{z}_b + T_y y + w\hat{\theta}, \tag{15}$$

where $\hat{\theta} \in \mathbb{R}^d$ is an on-line estimate of the parameter θ. The state estimation error verifies

$$\tilde{x} = w\tilde{\theta}. \tag{16}$$

Since, $w(t) > 0$ for all $t \in [0, \infty)$, the speed of convergence of the state estimator is *determined* by the speed of convergence of $\tilde{\theta}(t) \to 0$.

Remark 2. It is important to underscore that the proof of the lemma relies on the particular choice of initial condition for w given in (13). A discussion on the implications of this fact on the robustness of the design may be found in [28].

5.2. A parameterization suitable for parameter estimation

Lemma 3. Consider the system (1). There exists a matrix $N \in \mathbb{R}^{p\times m}$ such that the dynamics of the partial coordinate $y_a := Ny$ is given by

$$\dot{y}_a = -uy_a + r_a(y, x) + \xi_{ay}, \tag{17}$$

where $\xi_{ay} \in \mathbb{R}^p$ is measurable.

Proof. From (1) we get

$$\begin{aligned}\dot{y} &= L[-uc + Kr^0(c) + \xi] \\ &= -uy + LKQr(c) + L\xi \\ &= -uy + Sr_a(y,x) + L\xi,\end{aligned}$$

where we have used (5) in the second identity and, to obtain the third identity we used (8) and the fact that

$$\begin{aligned}LKQr(c) &= LP^{-1}\begin{bmatrix} I_p & 0_{p\times(q-p)} \\ 0_{(n-p)\times p} & 0_{(n-p)\times(q-p)}\end{bmatrix} r(c) \\ &= LP^{-1}\begin{bmatrix} r_a(y.x) \\ 0_{(n-p)}\end{bmatrix} \\ &= \begin{bmatrix} S & \star\end{bmatrix}\begin{bmatrix} r_a(y.x) \\ 0_{(n-p)}\end{bmatrix} \\ &= Sr_a(y,x)\end{aligned}$$

where $S \in \mathbb{R}^{m\times p}$. Under Assumption A1, S is a full-rank tall matrix and the proof is completed defining $N := S^\dagger$ and $\xi_{ay} := S^\dagger L\xi$

□□□

6. Reaction Rates Linear in the Unmeasurable State

When the reaction rates are linear in x the estimation of the vector θ reduces to the problem of identification of a *linearly parameterized* system. Indeed, replacing (11) in (17), we see that the dynamics of y_a takes the form

$$\begin{aligned}\dot{y}_a &= -uy_a + R(y)x + \xi_{ay} \\ &= -uy_a + \xi_{ay} + R(y)(T_{z_b}\hat{z}_b - T_y y + w\theta) \\ &= \Phi\theta + \xi_l \qquad (18)\end{aligned}$$

where we used (14) to get the second identity and, for the third identity, we defined the measurable signals

$$\begin{aligned}\xi_l &:= -uy_a + \xi_{ay} + R(y)(T_{z_b}\hat{z}_b - T_y y) \\ \Phi &:= R(y)w.\end{aligned}$$

Notice that (18) is *linear* in θ, therefore there are many ways to design an estimator for it. However, there exists a fundamental obstacle to ensure

its convergence. Indeed, from the definition of Φ above, and the fact that $w(t) \to 0$, we have that $\Phi(t) \to 0$—loosing identifiability of the parameter θ. In particular the matrix Φ *cannot satisfy* the well-known persistency of excitation condition

$$\int_t^{t+\kappa} \Phi^\top(s)\Phi(s)ds \geq \kappa I_d,$$

which is the necessary and sufficient condition for exponential convergence of the classical gradient and least-squares estimators [33, Theorem 2.5.1].

To overcome this obstacle we follow the estimator construction proposed in [18], which ensures *finite-time convergence* under a weak *sufficient excitation* assumption. To introduce the assumption and streamline the presentation of the observer, we define the following signals

$$\begin{aligned}
\dot{\Phi}_f &= -\lambda\Phi_f + \lambda\Phi \\
Y &= \frac{\lambda p}{p+\lambda} y_a - \frac{\lambda}{p+\lambda}\xi_l \\
\mathcal{Y} &= \mathrm{adj}\{\Phi_f^\top \Phi_f\}\Phi_f^\top Y \\
\Delta &= \det\{\Phi_f^\top \Phi_f\},
\end{aligned} \tag{19}$$

with $p := \frac{d}{dt}$, $\mathrm{adj}\{\cdot\}$ denotes the adjugate matrix and $\lambda > 0$ is a *free* tuning parameter.

Assumption A3 Fix two constants $\mu \in (0,1)$ and $\gamma > 0$. There exists $t_c > 0$ such that

$$\int_0^{t_c} \Delta^2(s)ds \geq -\frac{1}{\gamma}\ln(\mu).$$

Proposition 1. Consider the dynamics (18), (19) verifying Assumption A3 with the parameter estimator

$$\dot{\hat{\theta}} = -\gamma\Delta(\Delta\hat{\theta} - \mathcal{Y}), \tag{20}$$

and the state estimate

$$\hat{x} = T_{z_b}\hat{z}_b + T_y y + \frac{w}{1-v_c}[\hat{\theta} - v_c\hat{\theta}(0)], \tag{21}$$

where

$$v_c = \begin{cases} \mu & \text{if} \quad v \geq \mu \\ \\ v & \text{if} \quad v < \mu, \end{cases} \tag{22}$$

with v given by

$$\dot{v} = -\gamma\Delta^2 v, \quad v(0) = 1. \tag{23}$$

(i) The *individual* estimation errors are monotonically decreasing, that is,

$$|\tilde{\theta}_\ell(t_2)| \leq |\tilde{\theta}_\ell(t_1)|, \ \forall t_2 \geq t_1 \geq 0, \ \forall \ell \in \bar{d}.$$

(ii) The state observation error converges to zero in *finite-time*. More precisely,

$$\tilde{x}(t) = 0, \ \forall t \geq t_c.$$

Proof. Applying the filter $\frac{\lambda}{p+\lambda}$ to (18), and regrouping terms, we obtain the linear regression equation[4]

$$Y = \Phi_f \theta. \tag{24}$$

Multiplying this equation by $\text{adj}\{\Phi_f^\top \Phi_f\}\Phi_f^\top$, and recalling that $\text{adj}\{A\}A = \det\{A\}I_d$ for any—possibly singular—$d \times d$ matrix we obtain the identity

$$\mathcal{Y} = \Delta\theta, \tag{25}$$

where we underscore the fact that Δ is a *scalar*. Replacing this identity in (20), yields the parameter error equations

$$\dot{\tilde{\theta}}_\ell = -\gamma\Delta^2\tilde{\theta}_\ell, \ \forall \ell \in \bar{d},$$

The solution of these equations is given as

$$\tilde{\theta}_\ell(t_2) = e^{-\gamma\int_{t_1}^{t_2}\Delta^2(s)ds}\tilde{\theta}_\ell(t_1), \ \forall t_2 \geq t_1 \geq 0, \ \forall \ell \in \bar{d}, \tag{26}$$

from which the claim (i) follows immediately.

To prove (ii) notice that, from (23) and (26), we have that

$$\tilde{\theta}(t) = v(t)\tilde{\theta}(0).$$

Developing this equation leads to the key identity

$$[1 - v(t)]\theta = \hat{\theta}(t) - v(t)\hat{\theta}(0).$$

[4] As usual in adaptive control, we neglect an additive exponentially decaying term in (24) that is due to the filters initial conditions.

The proof is completed noting that, under Assumption A4, $v_c(t) = v(t)$ for all $t \geq t_c$. Consequently,

$$\frac{1}{1 - v_c}[\hat{\theta} - v_c\hat{\theta}(0)] = \theta, \ \forall t \geq t_c,$$

which implies that $\hat{x}(t) = x(t)$ for all $t \geq t_c$. □□□

Remark 3. We recall that Δ is the determinant of $\Phi_f^\top \Phi_f$, with Φ_f generated via LTI filtering of $R(y)w$. Since w is non-negative and SMD, Φ_f will tend to zero, which implies that also $\Delta(t) \to 0$—making Assumption A3 less stringent.

Remark 4. The signals $\mathcal{Y}$ and Δ are introduced to transform—via the operation of multiplication by $\text{adj}\{\Phi_f^\top \Phi_f\}\Phi_f^\top$—the ℓ-dimensional regression equation (24), into the ℓ *scalar* regressions given in (25). This step, known as "regressor mixing" was first introduced in the DREM estimator of [3], and has proven instrumental for the solution of many theoretical and practical problems, see [29] for a recent survey.

Remark 5. Although it is possible to design a high-gain observer [15] for the system $\dot{y}_a = -uy_a + R(y)x + \xi_{ay}$, this brings along the well-known problem of high sensitivity to noise [4, 35] that is unavoidable in reaction systems.

7. Reaction Rates Nonlinear in the Unmeasurable State

When the reaction rates are nonlinear in x the vector θ enters nonlinearly in the dynamics (17), giving rise to a difficult problem of estimation of a *nonlinearly parameterized* system, for which very little results are known. In this section we invoke the results of [23, 24], and exploit the SMI property of the reaction functions and Assumption A2 to design an asymptotically convergent I&I parameter estimator from the knowledge of the dynamics of y_a. As discussed in observation **O3** in Section 3, Assumption A2 is nedeed to ensure the SMI property, which is lost—in general—if the reaction functions contain products of different states x_ℓ.

The first step in the design is to notice that replacing the ℓ-th element of (14) in (12) we can define the functions $\psi_k : \mathbb{R} \times \mathbb{R}_+ \to \mathbb{R}_+$ as

$$\psi_k(\theta_\ell, t) := r_{k\ell}(e_\ell^\top [T_y y(t) + T_{z_b}\hat{z}_b(t)] + w(t)\theta_\ell)\mu_k(y(t)), \ k \in \bar{q}, \tag{27}$$

where $e_\ell \in \mathbb{R}^d$ is the ℓ-th vector of the Euclidean basis. We make the key observation that these functions are SMI with respect to the argument θ_ℓ. Indeed, by assumption, the functions $r_{k\ell}(x_\ell)$ are SMI. On the other hand, it is well-known that the *composition* of two SMI positive functions is also SMI, which is the scenario here since (14) is linear in θ_ℓ with positive "slope" w—hence is SMI.

Replacing (27) in (17), we see that the dynamics of the k-th component of the vector y_a is given as

$$\dot{y}_{ak} = -uy_{ak} + \psi_k(\theta_\ell, t) + \xi_{ayk}, \tag{28}$$

that is used as the basis for the design of our I&I parameter estimator given below.

Before presenting the main proposition we make the following important observation.[5] Since $\omega(t) \to 0$, the function (27) is not SMI with respect to θ_l *uniformly in time*. Therefore, we will be able to prove only *non-uniform* exponential convergence.

Proposition 2. Consider the dynamics (28) with the function $\psi_k(\theta_\ell, t)$ SMI in θ_ℓ. Define the I&I parameter estimator

$$\begin{aligned} \dot{\theta}_{I\ell} &= \gamma_\ell[uy_{ak} - \psi_k(\hat{\theta}_\ell, t) - \xi_{ayk}] \\ \hat{\theta}_\ell &= \gamma_\ell y_{ak} + \theta_{I\ell}, \ \ell \in \bar{d}, \end{aligned} \tag{29}$$

with $\gamma_\ell > 0$. Consider the Lyapunov function candidate $V_\ell(\tilde{\theta}_\ell) = \frac{1}{2}\tilde{\theta}_\ell^2$. Then, for any $T > 0$ there exists $\kappa = \kappa(T)$ such that

$$\dot{V}_\ell \leq -\kappa V_\ell, \tag{30}$$

for $t \leq T$.

Proof. Define the I&I estimate for the ℓ-th element of θ as

$$\hat{\theta}_\ell = \theta_{P\ell}(y_{ak}) + \theta_{I\ell}, \ \ell \in \bar{d}.$$

Computing its time derivative we get

$$\begin{aligned} \dot{\hat{\theta}}_\ell &= \dot{\theta}_{P\ell}(y_{ak}) + \dot{\theta}_{I\ell} \\ &= \theta'_{P\ell}(y_{ak})[-uy_{ak} + \psi_k(\theta_\ell, t) + \xi_{ayk}] + \dot{\theta}_{I\ell} \\ &= -\gamma_\ell[\psi_k(\hat{\theta}_\ell, t) - \psi_k(\theta_\ell, t)], \ \ell \in \bar{d}, \end{aligned}$$

[5]The authors thank an anonymous reviewer for pointing this essential fact to us.

where we have used (28) in the second equation, selected $\theta_{P\ell}(y_{ak}) = \gamma_\ell y_{ak}$ and replaced (29) to get the last identity.

Evaluating the derivative of the Lyapunov function candidate $V_\ell(\tilde{\theta}_\ell)$, we get

$$\dot{V}_\ell = -\gamma_\ell(\hat{\theta}_\ell - \theta_\ell)[\psi_k(\hat{\theta}_\ell, t) - \psi_k(\theta_\ell, t)] \leq -\kappa V_\ell, \tag{31}$$

where the last inequality follows from the SMI property of the function $\psi_k(\theta_\ell, t)$. □□□

Corollary 2. Consider the reaction system (1) verifying Assumptions A1 and A2. For the unmeasurable states *appearing* in (at least one of) the reaction functions define

$$\hat{x}_\ell = e_\ell^\top [T_y y(t) + T_{z_b} \hat{z}_b(t)] + w(t)\hat{\theta}_\ell,$$

with $\hat{\theta}_\ell$ generated via (27) and (29). Then, for any $T > 0$ there exists $\kappa = \kappa(T)$ such that

$$|\tilde{x}_\ell(t)| \leq \kappa e^{-\kappa t} |\tilde{x}_\ell(0)|, \ \forall t \leq T.$$

The unmeasurable states that *do not appear* in the reaction functions can be reconstructed from (9) and setting

$$\hat{x}_\ell = e_\ell^\top [T_y y(t) + T_{z_b} \hat{z}_b(t)]$$

which ensures[6]

$$|\tilde{x}_\ell(t)| = e^{-\int_0^t u(s)ds} |\tilde{x}_\ell(0)|, \ \forall t \geq 0.$$

□□□

Remark 6. For ease of presentation we have taken the simplest choice for the proportional term of the I&I estimator, namely $\theta_{P\ell}(y_{ak}) = \gamma_\ell y_k^\dagger$. As thoroughly discussed in [6, 24] this degree of freedom can be used to improve the transient performance. For instance, selecting

$$\theta_{P\ell}(y_{ak}) = \gamma_\ell y_{ak}^3,$$

and suitably redefining $\dot{\theta}_{I\ell}$, yields the bound $\dot{V}_\ell \leqslant -\kappa y_{ak}^2 V_\ell$.

Remark 7. From (31) it is clear that, if the function $\psi_k(\theta_\ell, t)$ is SMD—instead of SMI—it suffices to take $\gamma_\ell < 0$ to complete the proof of Proposition 2. On the other hand, if the function is *not strictly* monotonic, then only $\dot{V}_\ell \leqslant 0$ can be ensured.

[6] That is, the same convergence property of classical asymptotic observers [7].

8. Examples

In this section we illustrate with three benchmark examples the application, and performance improvement, of the proposed observers. In particular, for the non-isothermal chemical stirred tank reactor we present an *adaptive* observer that does not requires the knowledge of the parameters of the reaction function.

8.1. Stirred tank reactor with one microbial growth

Consider the stirred tank reactor with a simple microbial growth reaction with one substrate c_1 and one biomass c_2:

$$c_1 \to c_2,$$

studied in [30]. The typical observation question is then the estimation of biomass concentration c_2 from online measurements of c_1, that is, $y = c_1$ and $x = c_2$. Mass balances for both process components yields [30, eqs. (2) and (3)], which satisfy the model (1) with $n = 2,\ q = 1,\ m = 1,\ p = 1$ and the following definitions

$$K = \begin{bmatrix} -\frac{1}{k} \\ 1 \end{bmatrix},\ r^0(c) = R(c_1)c_2,\ \xi = \begin{bmatrix} uS_{in} \\ 0 \end{bmatrix},\ L = \begin{bmatrix} 1 & 0 \end{bmatrix},$$

where k, $R(c_1)$, u, S_{in}, c_1, c_2 represent the yield coefficient, the specific growth rate (h^{-1}), the dilution rate (h^{-1}), the influent substrate concentration (g/l), the substrate concentration in the reactor (g/l), and the biomass concentration in the reactor (g/l), respectively. The specific growth rate $R(c_1)$ is given by Monod or Haldane models, that is

$$R(c_1) = \begin{cases} R_{\max}\dfrac{c_1}{K_S + c_1} \\ R_{\max}\dfrac{c_1}{K_S + c_1 + \frac{c_1^2}{K_I}} \end{cases} \tag{32}$$

with $R_{\max}$ the maximum specific growth rate (h^{-1}), K_S the saturation constant (g/l) and K_I the inhibition constant (g/l). We assume that all terms and constants are known.

Notice that Assumption 1 is satisfied. To derive the dynamics required for the observer design, that is, (6) and (17), we define the matrices and constants

$$P = \begin{bmatrix} -1 & 0 \\ k & 1 \end{bmatrix},\ Q = k,\ W = I_2,\ T_{z_b} = 1,\ T_y = -k,\ N = -k$$

yielding

$$\begin{aligned}
\dot{y}_a &= -uy_a + R(y)x - k\xi_1 \\
\dot{z}_b &= -uz_b + k\xi_1 \\
x &= z_b + y_a \qquad (33)\\
y_a &= -ky. \qquad (34)
\end{aligned}$$

In this example x enters linearly, hence we can apply the observer proposed in Proposition 2. Moreover, noting that x—and consequently θ—are scalars, there is no need to generate the signals $\mathcal{Y}$ and Δ, see Remark 4. To highlight the performance improvement of the proposed observer, even without the inclusion of the finite-time convergence issue, we generate the observed state without this feature in the following.

Proposition 3. Consider the system (34), with the specific growth rate $R(y)$ given by (32), and the state observer

$$\begin{aligned}
\dot{\hat{z}}_b &= -u\hat{z}_b + k\xi_1 \\
\dot{w} &= -uw,\ w(0) = 1 \\
\dot{\Phi}_f &= -\lambda\Phi_f + \lambda R(y)w \\
Y &= \frac{\lambda p}{p+\lambda}y_a + \frac{\lambda}{p+\lambda}[k\xi_1 - R(y)y_a + uy_a - R(y)\hat{z}_b] \\
\dot{\hat{\theta}} &= -\gamma\Phi_f(\Phi_f\hat{\theta} - Y) \\
\hat{x} &= \hat{z}_b + y_a + w\hat{\theta}, \qquad (35)
\end{aligned}$$

with $\lambda > 0$ and $\gamma > 0$ *free* tuning parameters. The state observation error is given by

$$\tilde{x}(t) = e^{-\int_0^t [u(s)+\gamma\Phi_f^2(s)]ds}\tilde{x}(0). \qquad (36)$$

Denoting the state observation error of the *asymptotic observer* (9) as $\tilde{x}_{\texttt{AS}}$, we have

$$|\tilde{x}(t)| < |\tilde{x}_{\texttt{AS}}(t)|,\ \forall t > 0.$$

More precisely,

$$\tilde{x}(t) = e^{-\gamma\int_0^t \Phi_f^2(s)ds}\tilde{x}_{\texttt{AS}}(t). \qquad (37)$$

Proof. From Proposition 2 we get the parameter error equation

$$\dot{\tilde{\theta}} = -\gamma\Phi_f^2\tilde{\theta}.$$

The proof of (36) is completed invoking (16) and integrating (13) and the equation above.

To establish (37), we recall that the observation error of the asymptotic observer is given by (10). □□□

Simulation results for the proposed observer (35) and the asymptotic observer of [7] were carried out with the numerical values given in [30] with Monod's reaction $R(y) = 0.33\frac{y}{5+y}$ and $S_{in} = 5$. The tuning parameters were selected as $\lambda = 1$ and $\gamma = 100, 500, 5000$, with the initial conditions $x(0) = 2.05$, $y(0) = 0.9$ and all the other ones set to zero. Fig. 1 shows the behavior of $\tilde{x}$ and $\tilde{x}_{\mathtt{AS}}$, with the performance of the former been always better. As expected, increasing the adaptation gain γ yields a faster convergence, but an undershoot appears due to the time it takes for the various filters to effectively track their corresponding input signals. In Fig. 2 we repeat the previous simulation with $\gamma = 500$ and $\lambda = 1, 2, 10$. As predicted by the theory, increasing the bandwidth of the filter also reduces the convergence time but with a bigger undershoot.

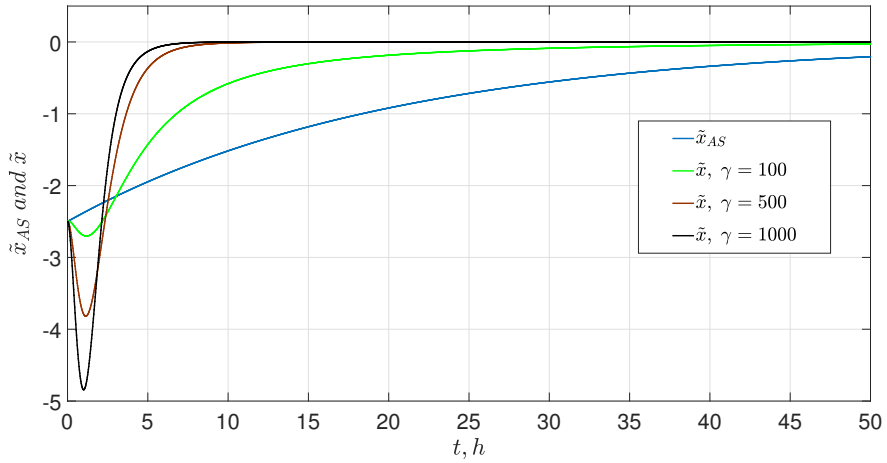

Figure 1: Transient behaviour of $\tilde{x}$ and $\tilde{x}_{\mathtt{AS}}$ with $\lambda = 1$ and $\gamma = 100, 500, 5000$

8.2. Non-isothermal chemical stirred tank reactor

We consider in this subsection a non-isothermal chemical stirred tank reactor with one reactant and one product

$$A \to bB,$$

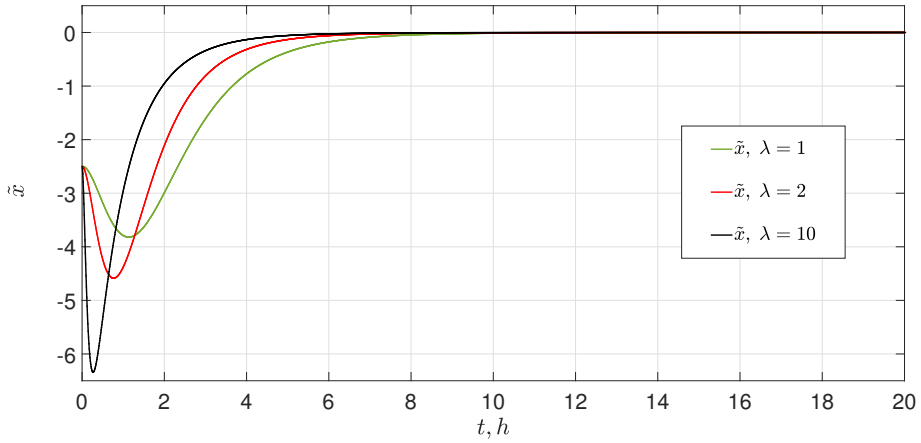

Figure 2: Transient behaviour of $\tilde{x}$ and $\tilde{x}_{\texttt{AS}}$ with $\gamma = 500$ and $\lambda = 1, 2, 10$

where b is the stiochiometric coefficient. The model dynamics of the process for the reactant concentration c_1, the product concentration c_2 and the temperature c_3 are readily derived from mass and energy balance considerations and lead to the set of differential equations given in [11, eqs. (2)-(4)]. This dynamics satisfy the model (1) with $n = 3$, $q = 1$, $m = 1$, $p = 1$ and the following definitions

$$K = \begin{bmatrix} -k_0 \\ bk_0 \\ k_0 \dfrac{\Delta H}{\rho C_p} \end{bmatrix}, \ r^0(c) = R(c_3)c_1,$$

$$\xi = \begin{bmatrix} uC_{in} \\ 0 \\ uT_{in} + \dfrac{hA}{\rho c_p V}(T - w - T) \end{bmatrix}, \ L = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix},$$

where k_0, E, R, q, V, C_{in}, T_{in}, ΔH, ρ, 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.

The typical observation question is the estimation of reactant concentration c_1 from online temperature of c_3, that is, $y = c_3$ and $x = c_1$. Notice that Assumption 1 is satisfied. To derive the dynamics required for the observer design, that is, (6) and (17), we define the matrices and constants

$$P = \begin{bmatrix} 0 & 0 & \frac{\rho C_p}{\Delta H} \\ b & 1 & 0 \\ -1 & 0 & \frac{\rho C_p}{\Delta H} \end{bmatrix}, \; Q = \frac{1}{k_0}, \; W = I_2, \; T_{z_b} = 1, \; T_y = -\frac{\rho C_p}{\Delta H}, \; N = -\frac{\rho C_p}{\Delta H}$$

yielding

$$\begin{aligned} \dot{y}_a &= -uy_a + R(y)x - \frac{\rho C_p}{\Delta H}\xi_3 \\ \dot{z}_b &= -uz_b - \frac{\rho C_p}{\Delta H}\xi_3 \\ x &= z_b + y_a \\ y_a &= -\frac{\rho C_p}{\Delta H}y. \end{aligned}$$

We consider two scenarios, when k_0 *is known* and when it is *not known*, in which case we propose a parameter estimator for it.

8.2.1. Known parameter k_0

In this case, we deal again with a system for which we can apply the observer of Proposition 2, which takes the form

$$\begin{aligned} \dot{\hat{z}}_b &= -u\hat{z}_b - \xi_3 \\ \dot{w} &= -uw, \; w(0) = 1 \\ \dot{\Phi}_f &= -\lambda\Phi_f + \lambda R(y)w \\ Y &= -\frac{\lambda p}{p+\lambda}y_a - \frac{\lambda}{p+\lambda}[\xi_3 - y_a[u + R(y)] - R\hat{z}_b] \\ \dot{\hat{\theta}}_1 &= -\gamma\Phi_f(\Phi_f\hat{\theta}_1 - Y). \end{aligned} \tag{38}$$

Notice that, since we are only interested in observing x_1, we have disregarded the dynamics of x_2 and $\hat{z}_2$. To incorporate the finite-time convergence feature we generate the state estimate as

$$\hat{x}_1 = \hat{z}_b + y_a + \frac{w}{1 - v_c}[\hat{\theta}_1 - v_c\hat{\theta}_1(0)],$$

where v_c is implemented via (22) and (23).

8.2.2. Estimation of the parameter k_0

The proposition below shows that it is possible to generate a linear scalar regression for the isolated parameter k_0. Consequently, with a construction similar to the one given in Proposition 1 it is possible to estimate it in *finite-time*, which can then be used in the observer (38) to generate an adaptive observer. For the sake of clarity the proof of the proposition is given in Appendix A.

Proposition 4. Consider the system

$$\dot{y}_{ak} = -uy_{ak} + k_0 R(y)x_1 + \xi_3. \tag{39}$$

There exists *measurable* signals $\mathcal{A}(t)$ and $\mathcal{B}(t)$ such that

$$\mathcal{A}(t) = \mathcal{B}(t)k_0. \tag{40}$$

8.3. Yeast growth

Yeast growth is one of the oldest industrial fermentation process. The following reaction network, with three growth reactions for the yeast, has been introduced in [34]:

- respirative growth on glucose : $c_1 + c_2 \to c_3 + c_4$;
- fermentative growth on glucose : $c_1 \to c_3 + c_4 + c_5$;
- respirative growth on glucose : $c_2 + c_5 \to c_3 + c_4$,

with c_1-c_5 denoting glucose, oxygen, yeast, CO_2, and ethanol, respectively.

The dynamics of the system is given by

$$\begin{aligned}
\dot{c}_1 &= u(c_{1,in} - c_1) - k_1\mu_1(c)c_3 - k_2\mu_2(c)c_3 \\
\dot{c}_2 &= -uc_2 + k_La(c_2^* - c_2) - k_4\mu_2(c)c_3 - k_3\mu_3(c)c_3 \\
\dot{c}_3 &= \mu_1(c)c_3 + \mu_2(c)c_3 + \mu_3(c)c_3 - uc_3 \\
\dot{c}_4 &= -uc_4 - k_v c_4 + k_5\mu_1(c)c_3 + k_6\mu_2(c)c_3 + k_7\mu_3(c)c_3 \\
\dot{c}_5 &= -uc_5 + k_8\mu_2(c)c_3 - k_9\mu_3(c)c_3
\end{aligned} \tag{41}$$

u, $c_{1,in}$, c_2^*, k_La and k_v are the dilution rate, the inlet glucose concentration, the oxygen saturation constant, and the liquid-gas transfer coefficients for oxygen and CO_2, respectively. k_i, $i = 1, \ldots, 9$, are yield coefficients. The

specific growth rates $\mu_i(c)$, $i = 1, 2, 3$, can be described by the following Monod models:

$$\mu(c) = \begin{bmatrix} \mu_{1,M} \frac{c_1}{k_{s1}+c_1} \frac{c_2}{k_{c2}+c_2} \\ \mu_{2,M} \frac{c_1}{k_{s2}+c_1} \\ \mu_{3,M} \frac{c_2}{k_{c1}+c_2} \frac{c_5}{k_{e5}+c_5} \end{bmatrix}$$

The system (41) can be rewritten in the form (1), with the definitions

$$\begin{aligned} & m = 5, q = 3, m = 3 \\ & K = \begin{bmatrix} -k_1 & -k_2 & 0 \\ 0 & -k_4 & k_3 \\ 1 & 1 & 1 \\ k_5 & k_6 & k_7 \\ 0 & k_8 & -k_9 \end{bmatrix}, \ \xi = \begin{bmatrix} uc_{1in} \\ k_L a(c_2^* - c_2) \\ 0 \\ k_v c_4 \\ 0 \end{bmatrix}, \\ & r(c) = c_3 \mu(c). \end{aligned}$$

Assuming that the measured quantities are c_2, c_4 and c_5, we can define $x := \text{col}(c_1, c_3)$ and $y := \text{col}(c_2, c_4, c_5)$. To derive the dynamics required for the observer design, that is, (6) and (17), we define the matrices P and Q

$$P = \begin{bmatrix} -(k_3 + k_4) & k_2 & -k_2 k_3 & 0 & 0 \\ k_3 & -k_1 & k_1 k_3 & 0 & 0 \\ k_4 & k_1 - k_2 & k_1 k_4 & 0 & 0 \\ P_{41} & P_{42} & -k_1(k_3 k_6 + k_4 k_7) - k_2 k_3 k_5 & 1 & 0 \\ P_{51} & P_{52} & -k_1 k_3 k_8 + k_1 k_4 k_9 & 0 & 1 \end{bmatrix},$$

$$Q = \begin{bmatrix} \frac{1}{k_1 k_3 + k_1 k_4 - k_2 k_3} & 0 & 0 \\ 0 & \frac{1}{k_1 k_3 + k_1 k_4 - k_2 k_3} & 0 \\ 0 & 0 & \frac{1}{k_1 k_3 + k_1 k_4 - k_2 k_3} \end{bmatrix},$$

$$W = I_5,$$

where

$$\begin{bmatrix} P_{41} & P_{42} \\ P_{51} & P_{52} \end{bmatrix} = \begin{bmatrix} k_3(k_5 - k_6) + k_4(k_5 - k_7) & k_1(k_6 - k_7) + k_2(k_7 - k_5) \\ -k_3 k_8 + k_4 k_9 & k_1 k_8 + k_1 k_9 - k_2 k_9 \end{bmatrix}$$

We make the important observation that $r_3(y, x)$ satisfies Assumption A3, allowing us to estimate x_2 from the dynamical system

$$\dot{y}_{a3} = -u y_{a3} + \mu_3(y_1, y_3) x_2 + \xi_{a3}.$$

Because of linearity in x_2, we can implement the observer with finite-time convergence of Proposition 2 to estimate it. Moreover, since this is a scalar equation, we don't need to generate the signals $\mathcal{Y}$ and Δ.

To estimate x_1 we can select the dynamics of y_{a2}, and write it as

$$\begin{aligned}\dot{y}_{a2} &= -uy_{a2} + \mu_{2,M}\frac{x_1}{k_{s2}+x_1}x_2 + \xi_{a2} \\ &= -uy_{a2} + \mu_{2,M}\frac{x_1}{k_{s2}+x_1}\hat{x}_2 + \xi_{a2} - \mu_{2,M}\frac{x_1}{k_{s2}+x_1}\tilde{x}_2,\end{aligned}$$

where we used $x_2 = \hat{x}_2 - \tilde{x}_2$ in the second equation. The key point here is that the fourth right hand in the latter equation converges to zero *in finite-time*. Therefore, it is possible to estimate x_1 applying the I&I observer of Proposition 2 with the dynamics

$$\dot{y}_{a2} = -uy_{a2} + \mu_{2,M}\frac{x_1}{k_{s2}+x_1}\hat{x}_2 + \xi_{a2},$$

which holds true for all $t \geq t_c$. For the sake of brevity, the details of these constructions are omitted here.

9. Conclusions and Future Work

It has been shown that, if knowledge on the reaction functions is available, we can design observers with improved convergence properties under the reasonable assumption of monotonicity. Of course, the main drawback of the approach is the well-known uncertainty on the parameters of the reaction functions. As shown in Subsubsection 8.2.2, in some particular examples it is possible to add an adaptation feature but, to date, we do not have a systematic procedure to do it for a general class of systems.

For the linear case, the reaction vector takes the form $r(y, x, \eta) = R(y, \eta)x$ where $\eta \in \mathbb{R}^p$ is a vector of uncertain parameters. If these parameters enter linearly, it is possible to propose an adaptation stage. In the nonlinear case, however, we would use in the observer of Proposition 1 and *a priori*, fixed estimate of η—say $\hat{\eta} \in \mathbb{R}^p$—and try to prove that if $\|R(y, \hat{\eta}) - R(y, \eta)\|$ is "small", the observer preserves some stability properties.

In the nonlinear case, we would need to add the following assumption to Proposition 2.

Assumption A4 A fixed, *a priori* estimate of η, denoted $\hat{\eta} \in \mathbb{R}^p$, is *known* such the following SMI-like property holds

$$(a-b)[r_{ak\ell}(a,\hat{\eta})\mu_k(y,\hat{\eta}) - r_{ak\ell}(b,\eta)\mu_k(y,\eta)] \geq \kappa|a-b|^2,\ \forall a,b \in \mathbb{R}_+,\ a \neq b. \tag{42}$$

□□□

Since in the case of *known* parameters, that is, $\hat{\eta} = \eta$, the SMI condition (42) reduces to

$$\mu_k(y)(a-b)[r_{ak\ell}(a) - r_{ak\ell}(b)] \geq \kappa|a-b|^2,\ \forall a,b \in \mathbb{R},\ a \neq b,\ \forall k \in \bar{q},$$

which is always true, it is clear that (42) holds—*locally* in x_ℓ—provided $|\hat{\eta}-\eta|$ is sufficiently small. Some preliminary calculations show, however, that the neighborhood for x_ℓ may be extremely small to be of practical interest.

[1] E. Aguilar-Garnica, J.P. Garcia-Sandoval and C. Gonzalez-Figueredo. A robust monitoring tool for distributed parameter plug flow reactors.. *Comp. Chem. Eng.*, vol 35, pp 510-518, 2011.

[2] J.M. Ali, N.H. Hoang, M.A. Hussain and D. Dochain. Review and classification of recent observers applied in chemical process systems. *Computers and Chemical Engineering*, vol. 76, no. 8, pp. 27-41, 2015.

[3] S. Aranovskiy, A. Bobtsov, R. Ortega and A. Pyrkin, Performance enhancement of parameter estimator via dynamic regressor extension and mixing, *IEEE Trans. Automatic Control*, vol. 62, no 7, pp.3546-3550, 2017.

[4] S. Aranovskiy, R. Ortega, J. Romero and D. Sokolov, A globally exponentially stable speed observer for a class of mechanical systems: experimental and simulation comparison with high-gain and sliding mode designs, *International Journal of Control*, vol. 92, no. 7, pp 1620-1633, 2019.

[5] A. Arshad Uppal, S. Siddique Butt, Q. Khan and H. Aschemann, Robust tracking of the heating value in an underground coal gasification process using dynamic integral sliding mode control and a gain-scheduled modified Utkin observer, *Journal of Process Control*, vol. 73, pp. 113-122, January 2019.

[6] A. Astolfi, D. Karagiannis and R. Ortega, *Nonlinear and Adaptive Control with Applications*, Springer, London, 2007.

[7] G. Bastin and D. Dochain, *On-line Estimation and Adaptive Control of Bioreactors*, Elsevier, Amsterdam, 1990.

[8] D. Bonvin, B. Srinivasan and D. Ruppen, Dynamic optimization in the batch chemical industry, *Preprints CPC6*, Tucson, Arizona, pp. 283-307, 2001.

[9] K. Chaib, A. Zemouche, M. Alma, H. Voos and M. Darouach, A Nonlinear observer-based trajectory tracking method applied to an anaerobic digestion process, *Journal of Process Control*, vol. 75, pp. 120-135, March 2019.

[10] H. De Battista, J. Pico, F. Garelli and A. Vignoni. Specific growth rate estimation in fed-batch bioreactors using second-order sliding observers. *Journal of Process Control*, vol 21, pp 1049-1055, 2011.

[11] D. Dochain, State and parameter estimation in chemical and biochemical processes: a tutorial, *Journal of Process Control*, vol. 13, no. 8, pp. 801-818, 2003.

[12] D. Dochain, *Automatic Control of Bioprocesses*, J. Wiley and sons, 2013.

[13] D. Dochain, M. Perrier and B.E. Ydstie. Asymptotic observers for stirred tank reactors. *Chem. Eng. Sci.*, vol 47, pp 4167-4177, 1992.

[14] F.J. Doyle III, Nonlinear inferential control for process applications, *Proc. ADCHEM'97*, pp. 170-181, 1997.

[15] F. Esfandiari and H. K. Khalil, Output feedback stabilization of fully linearizable systems, *Int. J. of Control*, vol. 56, pp. 1007-1037, 1992.

[16] M. Farza, K. Busawon, and H. Hammouri, Simple nonlinear observers for on-line estimation of kinetic rates in bioreactors, *Automatica*, vol. 34, no. 3, pp. 301-318, 1998.

[17] M. Farza, M. Oueder, R.B. Abdennour and M. Saad. High gain observer with updated gain for a class of MIMO nonlinear systems. *Int. J. Control*, vol. 84, pp 270-280, 2011.

[18] D. Gerasimov, R. Ortega and V. Nikiforov, Adaptive control of multivariable systems with reduced knowledge of high frequency gain: Application of dynamic regressor extension and mixing estimators, *18th IFAC Symposium on System Identification, (SYSID 2018)*, Stockholm, Sweden, July 9-11, 2018.

[19] N. Hoang, F. Couenne, Y. Le Gorrec, C.L. Chen and E. Ydstie, Passivity-based nonlinear control of CSTR via asymptotic observers, *Annual Reviews in Control*, vol. 37, pp 278-288, 2013.

[20] C. Kravaris, J. Hahn and Y. Chu, Y, Advances and selected recent developments in state and parameter estimation. *Computers and Chemical Engineering*, vol. 51, pp. 111-123, 2013.

[21] F. Lafont, E. Busvelle and J.P. Gauthier. An adaptive high-gain observer for wastewatertreatment systems. *J. Process Control*, vol. 21, pp 893-900, 2011.

[22] P. Lancaster and M. Tismenetsky, *The Theory of Matrices*, Academic Press, NY, 1985.

[23] X. Liu, R. Ortega, H. Su and J. Chu, Immersion and invariance adaptive control of nonlinearly parameterized nonlinear systems, *IEEE Trans. Automatic Control*, vol. 55, vo. 9, pp. 2209-2214, 2010.

[24] X. Liu, R. Ortega, H. Su and J. Chu, On adaptive control of nonlinearly parameterized nonlinear systems: Towards a constructive procedure, *Systems and Control Letters*, vol. 10, pp. 36-43, 2011.

[25] A. Mesbah, A.E.M. Huesman, H.J.M. Kramer and P.M.J. Van den Hof. A comparison of nonlinear observers for output feedback model-based control of seeded batch crystallization *J. Process Control*, vol. 21, pp 652-666, 2011.

[26] J. Moreno and D. Dochain, Global observability and detectability analysis of uncertain reaction systems and observer design, *International Journal of Control*, vol. 81, no. 7, pp. 1062-1070, 2008.

[27] P. Moya, M. Netto, R. Ortega, L. Praly and J. Pico: Application of nonlinear time-scaling for robust controller design for reaction systems, *Int. J. Robust and Nonlinear Control*, vol. 12, pp. 57-69, 2002.

[28] R. Ortega, A. Bobtsov, A. Pyrkin and A. Aranovskiy, A parameter estimation approach to state observation of nonlinear systems, *Systems and Control Letters*, vol. 85, pp 84-94, 2015.

[29] R. Ortega, S. Aranovskiy, A. Pyrkin, A Astolfi and A. Bobtsov: New results on parameter estimation via dynamic regressor extension and mixing: continuous and discrete-time cases, *IEEE Trans. Automatic Control*, (to be published).

[30] A. Rapaport and D. Dochain, Interval observers for biochemical processes with uncertain kinetics and inputs, *Mathematical Biosciences*, vol. 193, pp. 235-253, 2005.

[31] E. Rocha-Cozatl and A. Vande Wouwer. State and input estimation in phytoplanktonic cultures using quasi-unknown input observers. *Chem. Eng. J.*, vol. 175, pp 39-48, 2011.

[32] I. Sala-Mira, J. Diez, B. Ricarte and J. Bondia, Sliding-mode disturbance observers for an artificial pancreas without meal announcement *Journal of Process Control*, Vol. 78, pp. 68-77, June 2019.

[33] S. Sastry and M. Bodson, *Adaptive Control: Stability, Convergence and Robustness*, Prentice Hall, Englewood Cliffs, NJ, 1989.

[34] B. Sonnleitner and O. Kappeli, O., Growth of Saccharomyces cerevisiae is controlled by its limited respiratory capacity: formulation and verification of a hypothesis, *Biotechnol. Bioeng.*, vol. 18, pp. 927-937, 1986.

[35] B. Yi, R. Ortega and W. Zhang: On state observers for nonlinear systems: A new design and a unifying framework, *IEEE Trans. Automatic Control*, vol. 64, vo. 3, pp. 1193-1200, 2019.

Appendix A. Proof of Proposition 4

Replacing (14) in (39) we obtain

$$\begin{aligned}\dot{y}_{ak} &= -uy_{ak} + k_0 R(y)(T_{z_b}\hat{z}_b + y_{ak} + w\theta_1) + \xi_3 \\ &= \Phi_a k_0 \theta_1 + \Phi_b k_0 + \xi_a,\end{aligned}$$

where we defined the measurable signals

$$\Phi_a := R(y)w,\ \Phi_b := R(y)(T_{z_b}\hat{z}_b + y_{ak}),\ \xi_a := -uy_{ak}r + \xi_3.$$

Applying the filter $\frac{\lambda}{p+\lambda}$ to the equation above, and regrouping terms, yields the linear regression equation

$$Y_a = \Phi_{af}k_0\theta_1 + \Phi_{bf}k_0, \tag{A.1}$$

where

$$Y_a = \frac{\lambda p}{p+\lambda}y_{ak} - \frac{\lambda}{p+\lambda}\xi_a,\ \Phi_{af} = \frac{\lambda}{p+\lambda}\Phi_a,\ \Phi_{bf} = \frac{\lambda}{p+\lambda}\Phi_b.$$

Applying again the filter $\frac{\lambda}{p+\lambda}$ to (A.1) yields

$$Y_{af} = \Phi_{aff}k_0\theta_1 + \Phi_{bff}k_0,$$

where

$$Y_{af} = \frac{\lambda}{p+\lambda}Y_a,\ \Phi_{aff} = \frac{\lambda}{p+\lambda}\Phi_{af},\ \Phi_{bff} = \frac{\lambda}{p+\lambda}\Phi_{bf}.$$

The proof is completed defining the signals

$$\begin{aligned}\mathcal{A} &:= \Phi_{aff}Y_a - \Phi_{af}Y_{af}\\ \mathcal{B} &:= \Phi_{aff}\Phi_{bf} - \Phi_{af}\Phi_{bff}.\end{aligned}$$

which satisfy (40).