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A globally convergent estimator of the parameters of the classical model of a continuous stirred tank reactor

Anton Pyrkin [a,b,1], Alexey Bobtsov [b,1], Romeo Ortega [c,b,1], Jose Guadalupe Romero [c,*,1], Denis Dochain [d,1]

[a] HDU-ITMO Joint Institute, Hangzhou Dianzi University, Hangzhou, Zhejiang, PR China
[b] Department of Control Systems and Robotics, ITMO University, Kronverkskiy av. 49, Saint Petersburg, 197101, Russia
[c] Departamento de Ingeniería Eléctrica y Electrónica, ITAM, Rio Hondo, 1, Ciudad de México, 01080, Mexico
[d] ICTEAM, Université Catholique de Lovain, Avenue Georges Lemâitre 4-6, 1348 Louvain-la-Neuve, Belgium

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ABSTRACT

In this paper we provide the first solution to the challenging problem of designing a *globally convergent* estimator for the parameters of the standard model of a continuous stirred tank reactor. Because of the presence of *non-separable* exponential nonlinearities in the system dynamics that appear in Arrhenius law, none of the existing parameter estimators is able to deal with them in an efficient way and, in spite of many attempts, the problem was open for many years. To establish our result we propose a novel procedure to obtain a suitable *nonlinearly parameterized* regression equation and introduce a *radically new* estimation algorithm—derived applying the Immersion and Invariance methodology—that is applicable to these regression equations. A further contribution of the paper is that parameter convergence is *exponential* and is guaranteed with weak excitation requirements. To achieve this remarkable property we rely on the utilization of a recently introduced parameter estimator that seamlessly combines a classical least-squares search with the dynamic regressor extension and mixing estimation procedure.

1. Introduction

The non-adiabatic continuous stirred tank reactor (CSTR) is a common chemical and biochemical system in the process industry, and it is described extensively in [1,2]. To comply with the modern stringent monitoring and control requirements it is necessary to dispose of a reliable model, see [3] for a tutorial on their control and parameter estimation. Unfortunately, the dynamics of CSTRs is described by differential equations with highly uncertain parameters and, in particular, containing parameter-dependent *exponential terms* appearing in Arrhenius law that describes the behavior of the reaction rate. Since these nonlinearities are *not separable*, that is, they cannot be expressed as a product of a function of measurable signals and a function depending only on the parameters, none of the existing parameter estimation techniques is applicable to them. See [4] for a recent review of the existing approaches to solve this kind of problems.

The main contribution of this paper is to provide the first *globally convergent* estimator for the parameters of a CSTR assuming *known* only the kinetic constant appearing in Arrhenius law. The estimated parameters converge exponentially fast to their *true value* and the speed of convergence can be made arbitrarily fast increasing the adaptation gain in the estimator. Towards this end, we introduce a novel procedure to obtain a suitable nonlinearly parameterized regression equation (NLPRE) and—applying the Immersion and Invariance (I&I) methodology [5]—propose a *radically new* estimation algorithm applicable to these regression equations. An additional contribution of the paper is the fact that parameter convergence is guaranteed with extremely weak excitation requirements—namely *interval excitation* [6].

We underscore the fact that to establish our result we do not assume that the parameters leave in known compact sets, that the nonlinearities satisfy some Lipschitzian properties, nor rely on injection of high-gain—via sliding modes of the use of fractional powers—or the use of complex, computationally demanding methodologies. Instead, we propose to design a classical on-line estimator whose dynamics is described by an ordinary differential equation given in a compact precise form.

* Corresponding author.
E-mail addresses: pyrkin@itmo.ru (A. Pyrkin), bobtsov@itmo.ru (A. Bobtsov), romeo.ortega@itam.mx (R. Ortega), jose.romerovelazquez@itam.mx (J.G. Romero), denis.dochain@uclouvain.be (D. Dochain).

[1] All authors contributed equally to the paper.

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Notation. $\mathbb{R}_+$ and $\mathbb{Z}_+$ denotes the positive real and integer numbers, respectively, and $\mathbb{R}^n_+$ the set of n-dimensional vectors whose elements are all positive. For a column vector $a = \mathrm{col}(a_1, a_2, \dots, a_n) \in \mathbb{R}^n$, we denote $|a|^2 := a^\top a$ and define $a_{i,j} := \mathrm{col}(a_i, a_{i+1}, \dots, a_j)$, for $i, j \in \mathbb{Z}_+$, with $j > i$. For a matrix $A \in \mathbb{R}^{n\times m}$ we use $\|A\|$ for its Euclidean norm and denote its elements as A_{ij}. The action of a linear time-invariant (LTI) filter $\mathcal{H}(p) \in \mathbb{R}(p)$, with p the derivative operator, *i.e.*, $p(u) =: \frac{du(t)}{dt}$, on a signal $u(t)$ is denoted as $\mathcal{H}(p)(u)$. To simplify the notation, the arguments of all functions and mappings are written only when they are first defined and are omitted in the sequel.

2. System model and main result

We consider in the paper a non-isothermal CSTR with one reactant for which mass and energy balance considerations lead to the following differential equations [3,7]:

$$\dot{C}_A = \frac{q}{V}(C_{in} - C_A) - k_0 e^{-\frac{E}{RT}} C_A \tag{1a}$$

$$\dot{T} = \frac{q}{V}(T_{in} - T) - \frac{\Delta H}{\rho C_p} k_0 e^{-\frac{E}{RT}} C_A + \frac{hA}{\rho C_p V}(T_w - T) \tag{1b}$$

where the system states $C_A(t) \in \mathbb{R}_+$ and $T(t) \in \mathbb{R}_+$ are the concentration of the product and temperature, respectively. $T_w(t) \in \mathbb{R}_+$ is the heat exchanger temperature, that is an *input* signal and $T_{in}(t) \in \mathbb{R}_+$ is the influent temperature. The positive parameters[2]

$$\{E, R, q, V, C_{in}, \Delta H, \rho, C_p, h, A\},$$

whose physical meaning may be found in [2,3], are *unknown*. Notice that the only parameter assumed known is k_0, which is the kinetic constant appearing in Arrhenius law.[3]

We find convenient to rewrite the model in the more compact form

$$\dot{C}_A = \theta_1 - \theta_2 C_A - k_0 e^{-\frac{\theta_5}{T}} C_A \tag{2a}$$

$$\dot{T} = \theta_2(T_{in} - T) - \theta_3 k_0 e^{-\frac{\theta_5}{T}} C_A + \theta_4 u \tag{2b}$$

where we defined

$$\theta := \mathrm{col}\left(\frac{q}{V}C_{in}, \frac{q}{V}, \frac{\Delta H}{\rho C_p}, \frac{hA}{\rho C_p V}, \frac{E}{R}\right) \in \mathbb{R}^5,$$

and the new input

$$u := T_w - T.$$

Our task is to generate a *globally convergent estimate* of the parameters θ. To provide a solution to this problem we need the following.

Assumption 1. The system states C_A, T and the influent temperature T_{in} are *measurable*.

The main result of the paper is contained in the following proposition.

Proposition 1. *Consider the CSTR model (2a) verifying Assumption 1. There exists an on-line parameter estimator of the form*

$$\dot{\chi} = F_\chi(\chi, C_A, T, T_{in}, u)$$

$$\hat{\theta} = H_\chi(\chi, C_A, T, T_{in}, u)$$

with $\chi(t) \in \mathbb{R}^{n_\chi}$, such that for all $(C_A(0), T(0)) \in \mathbb{R}^2_+$, $\chi(0) \in \mathbb{R}^{n_\chi}$ and all continuous $u(t) \in \mathbb{R}$ that generates a bounded state trajectory, we ensure that all signals are bounded and the parameter estimation error $\tilde{\theta} := \hat{\theta} - \theta$ satisfies

$$\lim_{t\to\infty} |\tilde{\theta}(t)| = 0, \tag{3}$$

and the convergence is exponentially fast.

[2] The parameter ΔH—and consequently θ_3—are negative for exothermic reactions, while all the other parameters are positive.

[3] It is argued in [8] that, in practice, it is possible to estimate this coefficient from bench scale experiments.

3. Proof of Proposition 1

The proof proceeds in two steps, which are described in the following two subsections. First, the construction of an *overparameterized* linear regression equation (LRE) for the parameters $\theta_{1,4}$ and their consistent estimation with the least-squares plus dynamic regressor extension (LS+DREM) estimation algorithm reported in [9,10]. Second, the creation of a NLPRE for the remaining parameter θ_5 and their estimation with a *radically new* estimation procedure based on the I&I methodology.

3.1. Estimation of $\theta_{1,4}$

First, we eliminate the exponential term combining Eqs. () as

$$\theta_3\dot{C}_A - \dot{T} = \theta_1\theta_3 - \theta_2\theta_3 C_A - \theta_2(T_{in} - T) + \theta_4(-u), \tag{4}$$

that we rearrange as

$$-\dot{T} = \theta_1\theta_3 + \theta_2(T - T_{in}) + \theta_3(-\dot{C}_A) + \theta_4(-u) + \theta_2\theta_3(-C_A).$$

Fix a constant $\lambda > 0$ and apply the LTI, first order filter $\frac{\lambda}{p+\lambda}$, with $p := \frac{d}{dt}$, to the previous equation to get the following overparameterized LRE

$$y = \eta^\top \varphi + \varepsilon_t \tag{5}$$

where we defined

$$y := \frac{\lambda p}{p+\lambda}(-T),$$

the parameter vector

$$\eta := \mathrm{col}(\theta_1\theta_3, \theta_2, \theta_3, \theta_4, \theta_2\theta_3) \in \mathbb{R}^5, \tag{6}$$

and the regressor vector signal

$$\varphi := \mathrm{col}\left((1-\varepsilon_t), \frac{\lambda}{p+\lambda}(T - T_{in}), \frac{\lambda p}{p+\lambda}(-C_A), \frac{\lambda}{p+\lambda}(-u), \frac{\lambda}{p+\lambda}(-C_A)\right) \tag{7}$$

where ε_t is a *generic exponentially decaying signal*, which is neglected in the estimator equations.

To estimate the parameters of the LRE (5) we impose the *necessary* assumption that it is *identifiable* [11]. That is, that there exists a set of time instants—$\{t_i\}, i = 1 \dots, 5,\ t_i \in \mathbb{R}_{>0}$, such that

$$\mathrm{rank}\left\{ [\varphi(t_1)|\varphi(t_2)| \cdots |\varphi(t_5)] \right\} = 5.$$

We recall the following result of [12].

Lemma 1. *The LRE (5) is identifiable if and only if the regressor vector φ is interval exciting (IE) [6]. That is, there exist constants $c_c > 0$ and $t_c > 0$ such that*

$$\int_0^{t_c} \varphi(s)\varphi^\top(s)ds \ge c_c I_5.$$

The estimator we propose below consistently estimates the parameters $\eta_{1,4}$ of the LRE (5). It is clear from (6) that this yields the estimates of $\theta_{2,4}$, which are equal to $\eta_{2,4}$. On the other hand, to estimate θ_1 we need to compute it via

$$\hat{\theta}_1 = \frac{\hat{\eta}_1}{\hat{\eta}_3}. \tag{8}$$

It will be shown below that the monotonicity property of each parameter estimation error of DREM estimators avoids the possibility of a division by zero in (8).

We are in position to present the main result of the subsection whose proof relies on the following.

Assumption 2. The regressor φ given in (7) is IE.

Proposition 2. *Consider the LRE (5) verifying Assumption 2. Define the LS+DREM interlaced estimator with time-varying forgetting factor*

$$\begin{aligned}\dot{\hat{\mu}} &= \alpha F\varphi(y-\varphi^\top\hat{\mu}),\ \hat{\mu}(0)=:\ \mu^0\in\mathbb{R}^5\\ \dot{F} &= -\alpha F\varphi\varphi^\top F+\beta F,\ F(0)=\frac{1}{f_0}I_5\\ \dot{\hat{\eta}}_{1,4} &= \gamma_a\Delta(\mathcal{Y}_{1,4}-\Delta\hat{\eta}_{1,4}),\ \hat{\eta}_{1,4}(0)=:\ \eta^0_{1,4}\in\mathbb{R}^4_+\\ \dot{z} &= -\beta z,\ z(0)=1,\end{aligned}$$

where we defined

$$\begin{aligned}\beta &:= \beta_0\Big(1-\frac{\|F\|}{M}\Big)\\ \Delta &:= \det\{I_5-zf_0F\}\\ \mathcal{Y} &:= adj\{I_5-zf_0F\}[\hat{\mu}-zf_0F\mu^0],\end{aligned}$$

with tuning gains $\alpha>0,\ f_0>0,\ \beta_0>0,\ M\geq\frac{1}{f_0}$ and $\gamma_a>0$. Define the parameter estimates $\hat{\theta}_{2,4}=\hat{\eta}_{2,4}$ and $\hat{\theta}_1$ given by (8). Then, for all $f_0>0$, η^0_1 and $\theta^0_{2,4}$, we have that

$$\lim_{t\to\infty}|\tilde{\theta}_{1,4}(t)|=0, \tag{9}$$

and the convergence is exponentially fast, with all signals bounded, where $\tilde{\theta}_{1,4}:=\hat{\theta}_{1,4}-\theta_{1,4}$ is the estimation error vector. Moreover, the convergence rate can be made arbitrarily fast increasing the gain γ_a.

Proof. The proof of parameter convergence follows immediately from Lemma 1 and [9, Corollary 1]. The proof that $\hat{\eta}_3(t)>0$ to avoid a singularity in the calculation of (8) follows from the fact that the parameter errors verify the *monotonicity* condition

$$|\tilde{\theta}_i(t_a)|\leq|\tilde{\theta}_i(t_b)|,\ \forall t_a\geq t_b\geq 0,\ i=2,3,4,$$

and the observation from (6) that $\eta_3=\theta_3$. □

3.2. Estimation of θ_5 assuming known $\theta_{2,4}$

As in the previous subsection we first need to express the parameter θ_5 in a suitable equation, which is now nonlinearly parameterized. Towards this end, we find convenient to rewrite (2b) in the compact form

$$\dot{T}=\zeta_1(\theta_2,\theta_4)-\zeta_2(\theta_3)e^{\theta_5\phi}, \tag{10}$$

with the definitions

$$\begin{aligned}\zeta_1(\theta_2,\theta_4) &:= \theta_2(T_{in}-T)+\theta_4 u\\ \zeta_2(\theta_3) &:= \theta_3 k_0 C_A\\ \phi &:= -\frac{1}{T}.\end{aligned}$$

We propose in the following lemma a *completely new* estimator for the parameter θ_5 of 10, which is obtained applying the I&I methodology [5]. For the sake of clarity, we present first a lemma for the *ideal* case where we assume that the parameters $\theta_{2,4}$ are known—denoting the signals of this estimator with $(\cdot)^\star$. Then, as a corollary we define the actual $\hat{\theta}_5$ that uses the signals $\hat{\theta}_{2,4}$ and, carrying a simple perturbation analysis to the scheme of the lemma, prove its convergence.

Lemma 2. *Consider 10 assuming known the parameters $\theta_{2,4}$—hence the signals ζ_1 and ζ_2 are known. Following the I&I methodology define the estimate of θ_5 as the sum of a proportional and an integral term as*

$$\hat{\theta}^\star_5=\rho_P(T)+\rho^\star_I, \tag{11}$$

where

$$\rho_P(T)=\gamma_b\ln(T) \tag{12a}$$

$$\dot{\rho}^\star_I=\gamma_b\left(\zeta_1-\zeta_2e^{\hat{\theta}^\star_5\phi}\right)\phi \tag{12b}$$

with γ_b a tuning gain such that $\gamma_b sign(\theta_3)>0$.[4] *Then, for all initial conditions $\rho^\star_I(0)\in\mathbb{R}$ we have that all signals are bounded and*

$$\lim_{t\to\infty}|\tilde{\theta}^\star_5(t)|=0,$$

and the convergence is exponentially fast, where $\tilde{\theta}^\star_5:=\hat{\theta}^\star_5-\theta_5$ is the parameter error of the ideal estimator. Moreover, the convergence rate can be made arbitrarily fast increasing the gain γ_b.

Proof. The dynamics of the parameter error is given by

$$\begin{aligned}\dot{\tilde{\theta}}^\star_5 &= \dot{\hat{\theta}}^\star_5\\ &= \dot{\rho}_P+\dot{\rho}^\star_I\\ &= \gamma_b\frac{1}{T}\dot{T}+\gamma_b\left(\zeta_1-\zeta_2e^{\hat{\theta}^\star_5\phi}\right)\phi\\ &= -\gamma_b(\zeta_1-\zeta_2e^{\theta_5\phi})\phi+\gamma_b\left(\zeta_1-\zeta_2e^{\hat{\theta}^\star_5\phi}\right)\phi\\ &= \gamma_b\zeta_2\left(e^{\theta_5\phi}-e^{\hat{\theta}^\star_5\phi}\right)\phi\\ &= \gamma_b\zeta_2\left(e^{(\hat{\theta}^\star_5-\tilde{\theta}^\star_5)\phi}-e^{\hat{\theta}^\star_5\phi}\right)\phi\\ &= \gamma_b\zeta_2e^{\hat{\theta}^\star_5\phi}\left(e^{-\tilde{\theta}^\star_5\phi}-1\right)\phi\\ &=:\ \gamma_b d\left(e^{-\tilde{\theta}^\star_5\phi}-1\right)\phi,\end{aligned}$$

where we defined the signal $d(t)\in\mathbb{R}_+$, that satisfies

$$d(t):=\zeta_2(t)e^{\hat{\theta}^\star_5(t)\phi(t)}>0,\ \forall t\geq 0.$$

To analyze the stability of the error equation consider the Lyapunov function candidate $V(\tilde{\theta}^\star_5)=\frac{1}{2}(\tilde{\theta}^\star_5)^2$, whose derivative yields

$$\begin{aligned}\dot{V} &= \gamma_b d\left(e^{-\tilde{\theta}^\star_5\phi}-1\right)\tilde{\theta}^\star_5\phi\\ &= -\gamma_b d\phi^2 Q(\tilde{\theta}^\star_5\phi)[\tilde{\theta}^\star_5]^2,\end{aligned}$$

where we defined the function

$$Q(z)=\begin{cases}1 & z=0\\ \dfrac{1-e^{-z}}{z} & z\neq 0.\end{cases} \tag{13}$$

It is easy to prove that this function satisfies

$$\begin{aligned}&Q(z)>0,\quad\forall z\neq 0\\ &z\ \text{bounded}\ \Rightarrow\ Q(z)\ \text{bounded}.\end{aligned}$$

From the fact that $\dot{V}\leq 0$ we conclude that $\tilde{\theta}^\star_5$ is bounded, this together with the fact that ϕ is bounded and bounded away from zero, allows us to conclude that there exists $\phi_{\tt min}>0$, $Q_{\tt min}>0$ and $d_{\tt min}>0$ such that

$$\phi(t)\geq\phi_{\tt min},\ Q(z(t))\geq Q_{\tt min},\ d(t)\geq d_{\tt min}.$$

Consequently

$$\dot{V}\leq -2\gamma_b d_{\tt min}\phi^2_{\tt min}Q_{\tt min}V.$$

from which we conclude the proof. □

3.3. Certainty equivalent estimation of θ_5

In this subsection we present the actual estimator of the parameter θ_5 that relies on the estimation of $\theta_{2,4}$ as explained in Proposition 2 and the *ad-hoc* application of the certainty-equivalent principle, that is, replacing the unknown parameters $\theta_{2,4}$ by their estimates $\hat{\theta}_{2,4}$.

To simplify the notation we define the signals

$$\hat{\zeta}_1:=\zeta_1(\hat{\theta}_2,\hat{\theta}_4),\ \hat{\zeta}_2:=\zeta_2(\hat{\theta}_3).$$

[4] This requirement is imposed because, as mentioned in Footnote 1, the parameter θ_3 is negative for exothermic reactions and, in the sequel, we will require $\gamma_b\theta_3>0$.

Proposition 3. *Consider the system representation (10). Assume known an upperbound $\theta_5^{\max} > 0$ on θ_5. Define the I&I estimator of θ_5 as the projection of the sum of a proportional and an integral term as*

$$\hat{\theta}_5 = \begin{cases} \rho_P(T) + \rho_I & |\rho_P(T) + \rho_I| < \theta_5^{\max} \\ \theta_5^{\max} sign(\rho_P(T) + \rho_I) & |\rho_P(T) + \rho_I| = \theta_5^{\max}. \end{cases} \tag{14}$$

where $\rho_P(T)$ is given in (12a)[5] *and*

$$\dot{\rho}_I = \gamma_b \left(\hat{\zeta}_1 - \hat{\zeta}_2 e^{\hat{\theta}_5 \phi}\right)\phi, \tag{15}$$

with $\gamma_b \theta_3 > 0$ and the estimated parameters $\hat{\theta}_{2,4}$ are generated as indicated in Proposition 2. Then, for all initial conditions

$$\rho_I(0) \leq \theta_5^{\max} - \rho_P(T(0)),$$

we have that all signals are bounded and the parameter error verifies

$$\lim_{t\to\infty} \tilde{\theta}_5(t) = 0,$$

and the convergence is exponentially fast.

Proof. First, we make the observation that, due to (9), we have that

$$\hat{\zeta}_i(t) - \zeta_i(t) = \epsilon_t,\ i = 1, 2,$$

where we recall that—to avoid the proliferation of symbols—ϵ_t denotes a *generic* exponentially decaying signal. Now, from the definitions above we have the following.

$$\dot{\hat{\theta}}_5 = \begin{cases} \dot{\rho}_P + \dot{\rho}_I & |\rho_P(T) + \rho_I| < \theta_5^{\max} \\ 0 & \text{otherwise}. \end{cases}$$

We analyze now the first case

$$\begin{aligned} \dot{\hat{\theta}}_5 &= \dot{\rho}_P + \dot{\rho}_I \\ &= -\gamma_b \phi\left(\zeta_1 - \zeta_2 e^{\theta_5 \phi}\right) + \gamma_b \phi\left(\hat{\zeta}_1 - \hat{\zeta}_2 e^{\hat{\theta}_5 \phi}\right) \\ &= -\gamma_b \phi(\zeta_1 - \hat{\zeta}_1) + \gamma_b \phi \zeta_2 e^{\theta_5 \phi} - \gamma_b \phi(\zeta_2 + \epsilon_t) e^{\hat{\theta}_5 \phi} \\ &= \epsilon_t + \gamma_b \phi \zeta_2 \left(e^{\theta_5 \phi} - e^{\hat{\theta}_5 \phi}\right) - \gamma_b \phi\left(e^{\hat{\theta}_5 \phi} \epsilon_t\right) \\ &= \gamma_b \zeta_2 e^{\hat{\theta}_5 \phi} \phi\left(e^{-\tilde{\theta}_5 \phi} - 1\right) + \epsilon_t. \end{aligned}$$

Defining the signal

$$r(t) := \zeta_2(t) e^{\hat{\theta}_5(t)\phi(t)},$$

which—due to the inclusion of the projector operator that ensures $\hat{\theta}_5$ is bounded—is bounded and satisfies $r(t) \geq r_{\min} > 0$, we can write the last error equation as

$$\dot{\tilde{\theta}}_5 = \gamma_b r \phi\left(e^{-\tilde{\theta}_5 \phi} - 1\right) + \epsilon_t.$$

Mimicking the analysis of the error equation for $\tilde{\theta}_5^\star$ in the proof of Lemma 2, but now with the Lyapunov function candidate $U(\tilde{\theta}_5) = \frac{1}{2}\tilde{\theta}_5^2$, we obtain the bound

$$\dot{U} \leq -2\gamma_b r_{\min} \phi_{\min}^2 Q_{\min} U + \epsilon_t,$$

from which, invoking the Comparison Lemma, we conclude the proof. □

4. Simulation results

In this section we present simulations of the proposed estimators using the parameters of Table 1, which are taken from [8].

The simulations where carried out under the following three considerations.

Table 1
Parameters of the system.

Symbol	Value	Symbol	Value
q	1 [m^3/h]	R	1.98589 [kcal/kg mol K]
V	1 [m^3]	ΔH	−5960 [kcal/kg mol]
k_0	3.5·10^7 [1/h]	ρC_p	480 [kcal/(m^{3}K)]
E	11850 [kcal/kg mol]	hA	145 [kcal/(K h)]
C_{in}	10 [kg mol/m^3]		

(i) The input signal T_w is chosen time-varying, such that it provides sufficient excitation to the system to ensure parameter convergence. Solid arguments about the use of sinusoidal input signals are presented in [13] for the particular case of process control systems and in [14] for general systems.
(ii) The temperature T_{in} is normally assumed constant, however in the simulations we consider—again, for excitation requirement—that it is subject to small step changes [8].
(iii) Although in practice, one can determinate the pre-exponential non thermal factor k_0 from bench scale experiments [8], we present simulations of the estimator of Proposition 2 considering that k_0 is wrongly estimated.

In all simulations the implementation of the estimator for θ_5 of Proposition 3 was done without the projection operator, which was unnecessary.

To evaluate the performances of both estimators we carry out simulations under different values of γ_a, different values of γ_b and the last one assuming that the factor k_0 is measurable with an error of up to ±20% with respect to its real value.

In all simulations we fix the temperature T_{in} as,

$$T_{in}(t) = \begin{cases} 297 & t \in [0, 7) \\ 299 & t \in [7, 12] \\ 298 & t > 12 \end{cases} \tag{16}$$

notice that the temperature changes are of very small amplitude. The initial conditions were taken as $C_A(0) = 0.5$, $T(0) = 120$, the initial values of the parameter estimators were taken as $\mu^0 = 0.1$, $\hat{\eta}_1^0 = \hat{\theta}_{2,4}^0 = -1$, $\rho_I(0) = 7800$. We chose the filter parameter as $\lambda = 1$ and the tuning gains of the estimator as $f_0 = 0.1$, $\alpha = 68.4$, $\beta_0 = 30.6$ and $M = 130.5$.

For the first simulation we propose

$$T_w(t) = 350 - 20\exp(-0.001t)\cos(4t), \tag{17}$$

and different values of γ_a. The transient behavior of the estimation errors for each γ_a is identified by the color in Fig. 1. For all adaptation gains the response is quite smooth and, as predicted by the theory, the rise time diminishes with increasing gains. Also, we notice that the response of $\hat{\theta}_5$ is significantly slower[6] than the other four parameters, which stems from the fact that—as discussed in Section 3.3—the correct estimation of $\hat{\theta}_5$ depends on the convergence to zero of $\tilde{\theta}_{1,4}$. Also, notice the presence of an unexpected small oscillation around 4hrs, that may be due to numerical inaccuracies. Other signals T_w were tested, *e.g.*, without exponential decay and different frequencies, observing a similar behavior in all cases.

To assess the effects of the adaptation gain γ_b an additional simulation was carried out fixing $\gamma_a = 1800$, T_{in} as (16) and T_w as (17). Notice that the behavior of the I&I estimator does not influence the estimates $\hat{\theta}_{1,4}$, for this reason, we only show the transient behavior of the estimation error $\tilde{\theta}_5$. Fig. 2 shows estimation error $\tilde{\theta}_5$ for different values of γ_b distinguished by the line color in the label of the figure.

Finally, we evaluated the effect in the I&I estimator of errors in the *a priori* fixed value of the thermal factor k_0. The simulation scenario

[5] Notice that the proportional term $\rho_P(T)$ is independent of the parameters.

[6] Notice the difference in time scales.

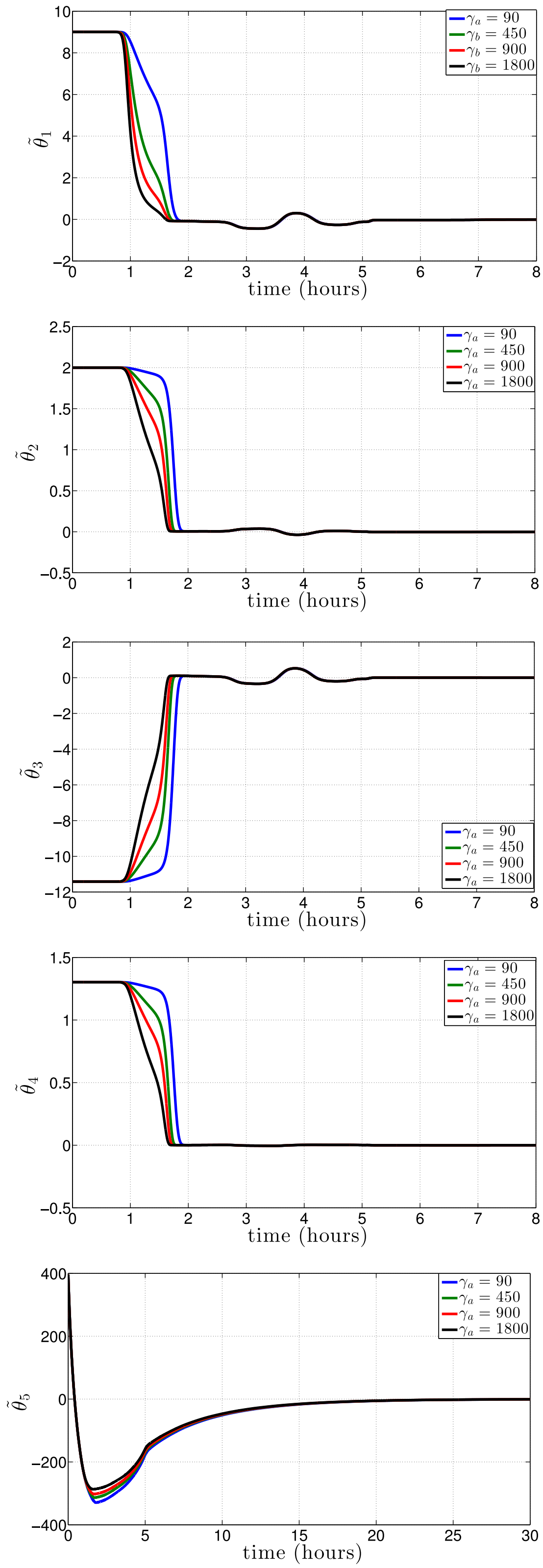

Fig. 1. Transient behavior of the estimation errors $\tilde{\theta}_{1,5}$ with different values γ_a and $T_w = 350 - 20\exp(-0.001t)\cos(4t)$.

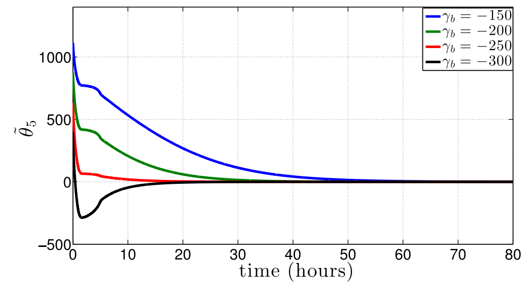

Fig. 2. Transient behavior of the estimation error $\hat{\theta}_5$ for different values of γ_b.

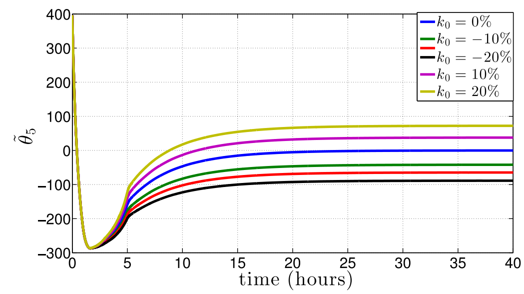

Fig. 3. Transient behavior of the estimation error $\hat{\theta}_5$ with incorrect values of k_0.

was the same as the one above. Fig. 3 presents $\tilde{\theta}_5$ assuming that k_0 has a measurable error, whose value is distinguished by the line color in the label of the figure. From the figure we see that the imprecise knowledge of k_0 induces a *steady-state bias* in the estimate, which increases with the size of the error on k_0.

5. Concluding remarks

We have presented in this paper the first solution to the problem of on-line estimation of the parameters of the classical model of a CSTR given in (1a) with the following assumptions:

- the reactor state—that is, the product concentration and the temperature—are measurable;
- the kinetic constant k_0 is known;
- the regressor vector (7) satisfies the (extremely weak) Assumption 2 of IE.

It is important to underscore the dramatic difference between IE and the assumption of *persistent excitation* (PE) [14, Section 2.5], usually invoked in state observation and identification problems. For instance, in [15] a dither signal, consisting of a large sum of sinusoids, is injected to the CSTR to enforce a PE assumption needed to ensure convergence of an extremum seeking controller. On the other hand, it is important to recall that PE endows the error equation of the estimation algorithm with the property of *exponential stability*, which is significantly stronger [16] than the property of exponential convergence established in Propositions 2 and 3

Model-free techniques have also been explored to address the present problem, without much success. For instance, in [17], a neural network technique is used to approximate the behavior of the CST, the authors require 1000 step changes (!) in the heat exchanger temperature to obtain a reasonable approximation—an experimental scenario that is utterly impractical.

Current research is under way to relax the assumption of *known* k_0 that, as shown in the simulations, induces a non-negligible steady-state error in the estimates. Notice that, with the definition $\theta_6 := \ln k_0$ it is possible to write (10) in the form

$$\dot{T} = \zeta_1 - \zeta_3 e^{\theta_{5,6}^\top \psi},$$

with the definitions

$$\zeta_3 := \theta_3 C_A,\ \psi := \begin{bmatrix} -\frac{1}{T} \\ 1 \end{bmatrix}.$$

Interestingly, mimicking the procedure of Lemma 2, it is possible to design an I&I estimator for $\theta_{5,6}$ that ensures $\lim_{t\to\infty} \tilde{\theta}_{5,6}^\top(t)\psi(t) = 0$, independently of the excitation properties of the vector ψ. Unfortunately, and rather surprisingly, it can be shown that the equilibrium associated to $\tilde{\theta}_{5,6} = 0$ is always *unstable*! Alternative designs of the estimator to overcome this problem are now being explored and we expect to be able to report them in the near future.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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