Robust Dynamic State Estimation of Nonlinear Plants

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An on-line state-estimation design for multiinput multioutput nonlinear plants, either observable or detectable, is presented. The design considers a stage of analysis, in which the solvability of the estimation problem with robust convergence is assessed a priori, and a stage of synthesis, in which the estimator is constructed and its gains are tuned with a systematized procedure. The approach, which stems from a suitable definition of robust nonlinear observability or detectability, provides a methodological framework that identifies the compromise between the performance and the robustness of the estimator and interprets the functioning of the estimator with notions and vocabulary from conventional-type linear filtering and control techniques. The problem for a class of free-radical homopolymerization reactors is studied as an application example showing how the proposed design, together with available nonlinear dynamics modeling and characterization methods, can be applied to polymer reactor engineering in particular and to chemical-process engineering in general.

Introduction

In process systems engineering, the problem of estimating the states of a nonlinear plant from its model in conjunction with its measured outputs constitutes an important problem, with applicability and implications in conventional and advanced feedback control, supervisory control, product quality monitoring, data reconciliation and failure detection, software sensors, the assistance of experimental designs intended for model validation or scale-up procedures, and so on. In particular, the applicability of a geometric (Alvarez, 1996) or a predictive (Phani and Bequette, 1996) model-based robust nonlinear control scheme depends on the functioning of a robust nonlinear estimator.

There are four main approaches to the design of nonlinear observers: (1) the extended Kalman filter (EKF) (Jazwinski, 1970), whose design is simple but lacks convergence criteria and systematic tuning procedures; (2) the geometric observer (GO) design (Bestle and Zeitz, 1983; Krener and Isidori, 1983; Krener and Respondek, 1985; Xia and Gao, 1989), which guarantees convergence with linear output error dynamics, but applies to an extremely restrictive class of plants; (3) the high-gain (HG) approach (Tsinias, 1989; Gauthier et al., 1992; Deza et al., 1992a, 1993; Ciccarella et al., 1993), which guarantees convergence, but has a complex tuning procedure; and (4) the sliding-mode (SM) approach (Slotine et al., 1987; Walcott et al., 1987), which guarantees robust stability, but has an elaborated design. The EKF, GO, HG, and SM techniques are restricted to nonlinear open-loop, observable plants (Krener and Respondek, 1985), and their extensions to partially observable (i.e., detectable) plants do not seem straightforward, as can be seen in the existence-oriented work of Tsinias (1990). Based on an observability or detectability requirement stated as a generalization of the assumptions made in Ciccarella et al.'s (1993) nominal observer design, Alvarez (1997, 1999) presented an estimator with a robust convergence criterion. For completely (Tornambe, 1992; Hammouri and Busawon, 1993; Alvarez, 1996) and partially (Alvarez, 1996) feedback-linearizable plants, HG-type estimators have been used to implement nonlinear geometric

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controllers with nominal stability, but cannot be applied to open-loop plants or to closed-loop plants with nongeometric controllers because the observability or detectability of a plant depends on the presence and the kind of feedback control.

In chemical engineering the EKF is by far the most widely used state estimation technique (Jo and Bankoff, 1976; Hyun et al., 1976; Schuler and Sushen, 1985; Schuler and Papadopoulou, 1986; Ellis et al., 1988, 1994; Dimitratos et al., 1991; Baratti et al., 1993, 1995), while the use of the GO, HG, and SD approaches is a recent and less widespread development (Kantor, 1989; Deza et al., 1992b, 1993; Van Dooting et al., 1992; Dochain et al., 1992; Wang et al., 1997). Furthermore, *ad hoc* (i.e., without convergence criteria) estimators have been tailored to implement nonlinear geometric controllers (Hoo and Kantor, 1985a,b; Kantor, 1989; Kravaris and Choung, 1987; Henson and Seaborg, 1991; Soroush and Kravaris, 1993; Daoutidis and Kravaris, 1994). Alvarez-Ramírez et al. (1997) used a closed-loop estimator in the robust nonlinear control of a class of chemical reactors. Soroush (1997) presented a nonlinear estimator for a class of detectable chemical reactors (Soroush, 1997; Tatirajou and Soroush, 1997), but its applicability has three problems: a verifiable test for detectability is lacking, a nonlinear gain must be constructed by inspection, and there is no convergence criterion.

Summarizing, nonlinear estimators have been used extensively in chemical engineering, and there is a growing interest in nonlinear designs with convergence criteria, but their acceptance and applicability require more systematic and clear designs, with contextualizations and interpretations beyond the mathematical-result format of the theoretical nonlinear estimation literature.

For multiinput multioutput (MIMO) nonlinear plants, either observable or detectable, in this work a robust state estimation design is presented that encompasses a broad range of systems in chemical engineering. The point of departure is Alvarez's (1997, 1999) robustly convergent P(proportional)-estimator, with a difference that is important in the application-oriented design here presented: while in the last work the estimability property was stated as a generalization of the one required in Ciccarella et al.'s (1993) nominally convergent observer design, here the estimability property is derived with a motivated constructive procedure. The proposed estimation design includes the two main and complementary stages that, according to the geometric method (Wonham, 1985), an engineering design must have: a stage of analysis where the concern is the *a priori* assessment of the solvability of the problem with a robust convergence criterion, and a stage of synthesis where the estimator is constructed and its gains are tuned with a systematized procedure. The systematization of the tuning of gains is accomplished with a pole-placement scheme that is similar to the ones used in the design of linear single-output filters and single-input controllers. As an option to improve the compensation of persistent disturbances induced by modeling errors, a PI(proportional-integral) version of the estimator is presented. The proposed design has a methodological framework that interprets the functioning of the estimator, and that exhibits the nature of its performance-robustness trade-off. The problem for a class of free-radical homopolymerization reactors is studied as an application example, showing how the estimation design can be assisted by standard nonlinear dynamic methods in polymer reactor engineering in particular, and in chemical process engineering in general.

Estimation Problem

Let us consider nonlinear plants

$$\dot{x} = f[x, u(t), r], \qquad x(t_o) = x_o, \qquad x_o \in X_o,$$
$$x \in X, \qquad r \in R \tag{1a}$$
$$y = h(x, r), \qquad u \in U, \qquad u(t) \in \mathfrak{U} \tag{1b}$$

with n states (x); m measured outputs (y); p known exogenous inputs (u); and n_r the model parameters (r). X_o and $\mathfrak{U}$ are the sets of admissible initial states and input trajectories $u(t)$. The input u, the state x, and the parameter r take values in the sets U, X, and R, respectively, that are compact (i.e., bounded and closed) due to physical and practical considerations. Each input $u_i(t)$ is a piecewise continuous function of time, and the maps f and h are sufficiently smooth (differentiable) in their respective domains. Thus, each set $\{x_o, u(t), r\}$ uniquely determines a (possibly unstable) state motion (Vidyasagar, 1978)

$$x(t) = \theta_x[t, t_o, x_o, u(t), r],$$

which in turn determines an output trajectory $y(t) = h[x(t), r]$.

The motion $x(t)$ of system 1a is said to be RE(robustly exponentially)-stable if there are four constants a_x, λ_x, b_u, and $b_r > 0$ so that, in some "tube" neighborhood of $x(t)$, the perturbed motions

$$\chi(t) = \theta_x[t, t_o, \chi_o, \hat{u}(t), \rho]$$

converge as follows:

$$\| \chi(t) - x(t) \| \leq a_x e^{-\lambda_x(t-t_o)} \| \chi_o - x_o \| + b_u \| \hat{u}(t) - u(t) \|^s$$
$$+ b_r \| \rho - r \|, \qquad \| \hat{u}(t) - u(t) \|^s = \sup_t \| \hat{u}(t) - \hat{u}(t) \|.$$

This definition of RE-stability implies Lyapunov ($\hat{u} = u$, $\rho = r$), bounded input−bounded output (BIBO) ($\chi_o = x_o$, $\rho = r$), and structural ($\chi_o = x_o$, $\hat{u} = u$) stability (Vidyasagar, 1978; Isidori, 1995). Essentially, RE-stability means that a perturbed motion $\chi(t)$ can stay arbitrarily close to the unperturbed motion $x(t)$ provided that it is made to start sufficiently close, with exogenous $[\hat{u}(t) - u(t)]$ and parameter $(\rho - r)$ errors that are kept sufficiently small.

Our problem consists of designing a dynamic state estimator,

$$\dot{\chi}_e = f_e[\chi_e, u(t), y(t), \rho], \qquad \chi_{eo} = \chi_e(t_0),$$
$$\chi = (I, 0)\chi_e, \qquad \chi_e = (\chi', \chi_a')', \qquad \dim \chi_e \geq \dim \chi,$$

built with a parameter approximation ρ of r, and such that, driven by the measured signals $u(t)$ and $y(t)$, it generates an inferred motion $\chi(t)$ that RE converges to the plant motion

$x(t)$. The state χ_e of the estimator includes the actual estimate χ of the plant, and can include an additional state χ_a to enable the processing of the measured input as well as the compensation of the persistent disturbance caused by the modeling error.

Estimability Property

In this section Alvarez's (1997, 1999) estimability property is derived with a constructive approach to the estimation problem, and presented in Definition 1. The P-estimator construction and its convergence criterion are presented in Theorem 1.

Auxiliary estimator

With an approach that stems from the proof of the sufficiency part of the well-known rank observability condition for linear plants (Kwakernaak and Sivan, 1972), let us consider the following auxiliary problem: assuming that the model parameters are known and that the measured signals are smooth functions of time, build an estimator using the measured signals and their time-derivatives, say

$$\boldsymbol{y}(t) = \left[y_1, \ldots, y_1^{(\kappa_1 - 1)}; \ldots; y_m, \ldots, y_m^{(\kappa_m - 1)} \right]'(t),$$
$$\kappa_1 + \cdots + \kappa_m = \kappa \leq n, \qquad \kappa_i > 0;$$
$$\boldsymbol{u}(t) = \left[u_1(t), \ldots, u_1^{(\nu_1 - 1)}; \ldots; u_p, \ldots, u_p^{(\upsilon_p - 1)} \right]'(t),$$
$$\nu_1 + \cdots + \nu_m = \nu \geq p, \qquad \nu_i > 0.$$

By taking successive time-derivatives of the output maps $h_1, \ldots, h_m$ (Eq. 1b) with substitutions of $\dot{x}$ by the right side of Eq. 1a, the following time-varying, algebraic, κ-equation set is obtained

$$\boldsymbol{y}(t) = \phi_{\mathrm{I}}[x, \boldsymbol{u}(t), r],$$
$$\phi_{\mathrm{I}}(x, \boldsymbol{u}, r) = \left[h_1, \ldots, L_f^{\kappa_1 - 1} h_1; \ldots; h_m, \ldots, L_f^{\kappa_m - 1} h_m \right]', \quad (2)$$

where ϕ_{I} is a nonlinear map, and $L^i_f \alpha$ denotes the recursive directional derivative of the time-varying scalar field $\alpha(x, t)$ along the time-varying vector field $f(x, t)$:

$$L_f^{i+1} \alpha = L_f\left(L_f^i \alpha \right), \qquad i \geq 1, \qquad L_f^0 \alpha = \alpha;$$
$$L_f \alpha = \alpha_x f + \alpha_t, \qquad \alpha_x = \partial \alpha / \partial x, \qquad \alpha_t = \partial \alpha / \partial t.$$

If Eq. 2 consists of $\kappa \leq n$ independent equations (Assumption 1, from now on "As. 1"), it establishes that the state of the plant is in the $(n - \kappa)$-dimensional surface

$$\Xi(t) = \left\{ x \in X \mid \phi_{\mathrm{I}}[x, \boldsymbol{u}(t), r] = \boldsymbol{y}(t) \right\},$$
$$0 \leq \dim \Xi = n - \kappa \leq n - m, \quad (3)$$

which is denominated unobservable because, unless $\kappa = n$, from Eq. 2 one cannot say where in $\Xi(t)$ the state x of the plant is. Accordingly, the restricted $(n - \kappa)$-dimensional system

$$\dot{x}^* = f[x^*, u(t), r], \qquad x^*(t_0) = x_o, \qquad x^*(t) \in \Xi(t):$$
$$x^*(t) = \theta_x^*[t, t_o, x_o, \boldsymbol{u}(t), \boldsymbol{y}(t), r] \quad (4)$$

and its motion $x^*(t)$ will be referred to as the unobservable dynamics and motion, respectively. The plant and its unobservable motions coincide [i.e., $x^*(t) = x(t)$], but the same is not necessarily true for their stability properties. If $x(t)$ is stable, $x^*(t)$ is stable. If $x(t)$ is unstable, $x^*(t)$ can be stable or unstable. If the unobservable motion $x^*(t)$ is E-stable (As. 2), the on-line integration of the auxiliary estimator

$$\dot{\chi} = f[\chi, u(t), r], \qquad \chi(t_0) = \chi_o \neq x_o \qquad \chi(t) \in \Xi(t) \quad (5)$$

yields a motion $\chi(t)$ that E-converges to the plant motion $x(t)$, according to the inequality

$$\| \chi(t) - x(t) \| \leq A_x \, e^{-L_{\mathrm{II}}(t - t_o)} \| \chi_o - x_o \|,$$
$$\chi(t), x(t) \in \Xi(t), \qquad (a_x, \lambda_{\mathrm{II}}) = \lim_{\chi \to x} (A_x, L_{\mathrm{II}}). \quad (6)$$

The auxiliary estimator (Eq. 5) (1) is made of n independent equations, with κ algebraic ones defining the unobservable surface $\Xi(t)$, and $n - \kappa$ differential ones describing the evolution of the inferred motion $\chi(t)$ in $\Xi(t)$; (2) cannot be implemented because it is improper (i.e., time derivatives of the measured signals are required); (3) sets the limiting estimator performance; and (4) is the first step in the construction of a proper estimator.

Proper estimator

A proper estimator is built next by making three modifications to the auxiliary estimator (Eq. 5): the maps f and h are evaluated with the approximated parameter ρ, the augmented input $\boldsymbol{u}$ is estimated with a linear filter (Eq. 8a), and the static restriction $\chi \in \Xi(t)$ (in Eq. 5) is replaced by an output-driven corrector $[G(y - h)$ in Eq. 8b].

First regard the augmented input $\boldsymbol{u}$ as the state x_u of a dynamic exosystem (Eq. 7a) driven by the bounded exogenous input $\upsilon(t)$, then introduce the augmented version of the plant (Γ_u, Π_u, and Δ_u are block-diagonal matrices defined in Appendix A)

$$\dot{x}_u = \Gamma_u x_u + \Pi_u \upsilon(t), \qquad u = \Delta_u x_u, \qquad \upsilon = \left[u_1^{(\nu_1)}, \ldots, u_p^{(\upsilon_p)} \right]',$$
$$\| \upsilon(t) \| \leq \epsilon_\upsilon \quad (7a)$$
$$\dot{x} = f(x, \Delta_u x_u, r), \qquad y = h(x, r), \quad (7b)$$

and finally consider the dynamic system

$$\dot{\chi}_u = \Gamma_u \chi_u + K_u(u - \Delta_u \chi_u), \qquad \psi_u = \Delta_u \chi_u \quad (8a)$$
$$\dot{\chi} = f(\chi, \Delta_u \chi_u, \rho) + G(\chi, \chi_u, \rho)[y - h(\chi, \rho)],$$
$$\psi = h(\chi, \rho) \quad (8b)$$

as a candidate estimator for the augmented plant (Eq. 7), where ψ_u and ψ are estimates of the measured signals, u and

y, and K_u (linear) and G (nonlinear) are gain matrices to be determined.

Error dynamics

Let us assume (As. 3) that there is a map $\phi_{\rm II}$ $(x,\ \boldsymbol{u},\ r)$ so that the map ($\phi_{\rm I}$ is defined in Eq. 2)

$$\phi(x,\ \boldsymbol{u},\ r) = [\phi_{\rm I}',\ \phi_{\rm II}']',$$
$$\phi^{-1}\{\phi[x(t),\ \boldsymbol{u}(t),\ r],\ \boldsymbol{u}(t),\ r\} = x(t)$$

is continuously differentiable for x and u and is Rx-invertible (robustly invertible for x) about $[x(t),\ \boldsymbol{u}(t),\ r]$, meaning that there is an inverse map ϕ^{-1}, and that ϕ and ϕ^{-1} are L(Lipschitz)-continuous, that is to say, that there are two sets $\{F_x,\ F_u,\ F_r\}$ and $\{D_z,\ D_u,\ D_r\}$ of positive constants so that, in some neighborhood of $[x(t),\ \boldsymbol{u}(t),\ r]$, ϕ and ϕ^{-1} are bounded by

$$\|\phi(\chi, \chi_u,\ \rho) - \phi(x,\ \boldsymbol{u},\ r)\| \le D_x\|\chi - x\| + D_u\|\chi_u - \boldsymbol{u}\| + D_r\|\rho - r\| \quad (9a)$$

$$\|\phi^{-1}(\zeta,\ \zeta_u,\ \rho) - \phi^{-1}(z,\ z_u,\ r)\| \le F_z\|\zeta - z\| + F_u\|\zeta_u - z_u\| + F_r\|\rho - r\|. \quad (9b)$$

Now subtract the augmented plant (Eq. 7) from its estimator (Eq. 8), apply the "straightening" error coordinate-change

$$e_u = \chi_u - x_u, \qquad e_{\rm I} = \phi_{\rm I}(\chi,\ \chi_u,\ \rho) - \phi_{\rm I}(x,\ x_u,\ r),$$
$$e_{\rm II} = \phi_{\rm II}(\chi,\ \chi_u,\ \rho) - \phi_{\rm II}(x,\ x_u,\ r), \quad (10)$$

set the nonlinear gain matrix (K_o is a gain matrix to be determined)

$$G = [\phi_x^{-1}(\chi,\ \chi_u,\ \rho)]\begin{bmatrix} K_o \\ 0 \end{bmatrix} \quad (11)$$

and obtain the following estimation error dynamics (the matrices A_u and A_o and the nonlinear maps ω, q_I, and $q_{\rm II}$ are defined in Appendix A)

$$\dot{e}_u = A_u e_u - \Pi_u \upsilon(t), \qquad \mu = \Delta_u e_u \quad (12a)$$

$$\dot{e}_{\rm I} = A_o e_{\rm I} + \Pi_o q_{\rm I}[e,\ e_u,\ \upsilon(t),\ e_r,\ t], \qquad \upsilon = \Delta_o e_{\rm I} \quad (12b)$$

$$\dot{e}_{\rm II} = \omega(e_{\rm II},\ t) + q_{\rm II}[e,\ e_u,\ \upsilon(t),\ e_r,\ t], \quad (12c)$$

where the observability of the matrix pairs $(\Gamma_u,\ \Delta_u)$ and $(\Gamma_o,\ \Delta_o)$ guarantee the existence of gain matrices K_u and K_o such that the matrices A_u and A_o, respectively, are stable. The choice of the matrix G (Eq. 11) has been dictated by the following considerations: (1) the unobservable error dynamics (Eq. 12c) must not have measurement injection [i.e., $(\partial\phi_{\rm II}/\partial x)G = 0$], and (2) the observable error dynamics Eq. 12b must be quasi-linear [i.e., $(\partial\phi_{\rm I}/\partial x)G = K_o$].

By construction, the error motions of the exo-observable (Eq. 12a) and of the unobservable (Eq. 12c) dynamics are RE-stable, and therefore, the boundedness (say L-continuity: As. 4) of the nonlinear disturbance $q_{\rm I}$ is necessary for the RE-stability of the observable error dynamics (Eq. 12b), and this in turn is a necessary condition for the RE-stability of the interconnected error dynamics (Eq. 12).

Estimability property

In the next definition, the four assumptions (As. 1, ..., As. 4) made in the construction of the candidate estimator (Eqs. 8 and 11) are listed and presented as the estimability property of the proposed estimation design.

Definition 1. The motion $x(t)$ of the plant (Eq. 1) is *RE(robustly exponentially)-estimable* if there are m integers (observability indices) $\kappa_1,\ \ldots,\ \kappa_m$ $(\kappa_1 + \cdots + \kappa_m = \kappa \le n,\ \kappa_i > 0)$ and a map $\phi_{\rm II}(x,\ \boldsymbol{u},\ r) = [\phi_{\kappa+1},\ \ldots,\ \phi_n]'$ such that, in some neighborhood about $[x(t),\ \boldsymbol{u}(t),\ r]$ (i.e., about the plant motion, the augmented input trajectory, and the parameter r):

(i) The map $\phi(x,\ \boldsymbol{u},\ r) = [\phi_{\rm I}',\ \phi_{\rm II}']'_{(x,\ \boldsymbol{u},\ r)}$ is Rx-invertible ($\phi_{\rm I}$ is defined in Eq. 2)

(ii) The map $\varphi(x,\ \boldsymbol{u},\ \upsilon) := [L_f^{\kappa_1}h_1;\ \ldots;\ L_f^{\kappa_m}h_m]'$ is L-continuous (υ is defined in Eq. 7a)

(iii) The unobservable motion $x^*(t)$ (Eq. 4) is RE-stable.

If $\kappa = n$ [i.e., there are no unobservable dynamics, and condition (iii) is trivially met] the motion $x(t)$ is said to be RE-observable. Otherwise, if $\kappa < n$, the motion $x(t)$ is said to be RE-detectable. The integers $\nu_1,\ \ldots,\ \nu_{\rm p}$ $(\nu_i > 0)$ are denominated exo-observability indices.

In a nonlinear nonautonomous system (i.e., with input u) the estimability is a property of a motion of the plant, which depends on a particular initial condition-input pair, and is independent of the construction-tuning stage. If the plant is autonomous, conditions (i) and (ii) are tested in the neighborhood of a steady-state (i.e., a time-invariant motion) $\bar{x}$, condition (iii) becomes the RE-stability of $\bar{x}$, and the estimability property holds for all the state motions in a neighborhood of $\bar{x}$. If the plant is linear and time-invariant, the nominal version of condition (i) with $\kappa = n$ coincides with the well-known rank observability condition (Kwakernaak and Sivan, 1972). With $\kappa < n$ and κ maximum, condition (ii) is trivially met, and conditions (i) and (iii) are the geometric definition of detectability (Basile and Marro, 1992). In Definition 1, the unobservable surface has not been required to be minimal in order to leave the choice of the observability index set $\boldsymbol{k} = \{\kappa_1,\ \ldots,\ \kappa_m\}$ as a degree of freedom in the design. Comparing with the HG observer designs, the nominal version of property (i) for the case of E-observability (i.e., $\kappa = n$) implies local observability at a state set (Hermann and Krener, 1977), uniform observability (Isidori, 1995), one of the solvability conditions of the GO design (Krener and Isidori, 1983), and one of the assumptions of the HG observer design (Gauthier et al., 1992; Ciccarella et al., 1993).

RE-convergence

In this section, a sufficient condition for the convergence of the P-estimator is presented. For this purpose let us first introduce various constructions and definitions related to the stability of the matrices A_u and A_o, and to the "sizes" of the disturbances $q_{\rm I}$ and $q_{\rm II}$ of the estimation error dynamics (Eq. 12).

Let the adjustable estimator gains have the parametrized form (Alvarez, 1996)

$$K_u(s_u) = bd\left[\left(s_u k_{11}^u, \ldots, s_u^{\nu_1} k_{\nu_1 1}^u\right)', \ldots, \left(s_u k_{1p}^u, \ldots, s_u^{\nu_p} k_{\nu_p p}^u\right)'\right], \quad s_u > 0 \quad (13a)$$

$$K_o(s_o) = bd\left[\left(s_o k_{11}^o, \ldots, s_o^{\kappa_1} k_{\kappa_1 1}^o\right)', \ldots, \left(s_o k_{1m}^o, \ldots, s_o^{\kappa_m} k_{\kappa_m m}^o\right)'\right], \qquad s_o > 0, \quad (13b)$$

with entries of $K_u(1)$ and $K_o(1)$ that set stable the reference linear, noninteractive and pole-assignable (LNPA) output error dynamics

$$\mu_i^{(\nu_i)} + k_{1i}^u \mu_i^{(\nu_i - 1)} + \cdots + k_{\nu_i i}^u \mu_i = 0, \qquad 1 \le i \le p; \qquad \mu_i = \psi_i^u - u_i \quad (14a)$$

$$\mathfrak{v}_i^{(\kappa_i)} + k_{1i}^o \mathfrak{v}_i^{(\kappa_i - 1)} + \cdots + k_{\kappa_i i}^o \mathfrak{v}_i = 0, \qquad 1 \le i \le m; \qquad \mathfrak{v}_i = \psi_i - y_i, \quad (14b)$$

so that the resulting parametrized matrices $A_u(s_u)$ and $A_o(s_o)$ [of the estimation error dynamics (Eq. 12)] meet the E-stability inequalities (Alvarez, 1996)

$$\| e^{tA_u(s_u)} \| \le a_u e^{-s_u \lambda_u t}, \qquad t \ge 0 \quad (15a)$$

$$\| e^{tA_o(s_o)} \| \le a_o e^{-s_o \lambda_o t}, \qquad t \ge 0, \quad (15b)$$

where the pairs (a_u, λ_u) and (a_o, λ_o) are set by $K_u(1)$ and $K_o(1)$, and are independent of s_u and s_o.

The L-continuous disturbances q_{I} and q_{II} of the error dynamics (Eq. 12) are bounded as follows

$$\| q_{\mathrm{I}}(e, \upsilon, e_r, t) \| \le M_u \| e_u \| + M_{\mathrm{I}} \| e_{\mathrm{I}} \| + M_{\mathrm{II}} \| e_{\mathrm{II}} \| + M_r \epsilon_r, \quad (16a)$$

$$\| q_{\mathrm{II}}(e, \upsilon, e_r, t) \| \le N_u \| e_u \| + N_{\mathrm{I}} \| e_{\mathrm{I}} \| + N_r \epsilon_r \quad (16b)$$

$$(m_{\mathrm{I}}, m_{\mathrm{II}}, n_{\mathrm{I}}) = \lim_{(e, e_r) \to 0} (M_{\mathrm{I}}, M_{\mathrm{II}}, N_{\mathrm{I}}) \quad (17)$$

and c_x^ϕ denotes the largest condition number, along the plant motion, of the Jacobian matrix ϕ_x of the estimability map ϕ of Definition 1. This is (D_x and F_z are defined in Eq. 9),

$$c_x^\phi = \lim_{(e, e_r) \to 0} C_x^\phi, \qquad C_x^\phi(N) = \sup_{(\chi, \chi_u, \rho) \in N} (D_x / F_z). \quad (18)$$

In the next theorem, a sufficient condition for the convergence of the P-estimator is presented, and the construction of the estimator is summarized.

Theorem 1 (Alvarez, 1997, 1999). Let the motion $x(t)$ of the plant (Eq. 1) be RE-estimable in the sense of Definition 1, and let the reference gains (Eq. 13), $K_u(1)$ and $K_o(1)$, make stable the reference LNPA output error dynamics (Eq. 14). Then, the P-estimator

$$\dot{\chi}_u = \Gamma_u \chi_u + K_u(s_u)(u - \Delta_u \chi_u), \qquad \psi_u = \Delta_u \chi_u \quad (19a)$$

$$\dot{\chi} = f(\chi, \Delta_u \chi_u, \rho) + G(\chi, \chi_u, \rho)[y - h(\chi, \rho)], \qquad \psi = h(\chi, \rho), \quad (19b)$$

with the parametrized gains (Eq. 13) $K_u(s_u)$ and $K_o(s_o)$, and the nonlinear gain

$$G(\chi, \chi_u, \rho) = \Theta_{\mathrm{I}}(\chi, \chi_u, \rho) K_o(s_o), \qquad [\Theta_{\mathrm{I}}, \Theta_{\mathrm{II}}] := \phi_x^{-1}(\chi, \chi_u, \rho) \quad (19c)$$

yields a motion $\chi(t)$ that RE-converges to $x(t)$ if the parameter s_o is chosen sufficiently large so that:

$$s_o \lambda_o > a_o m_{\mathrm{I}} \quad \text{if} \quad \kappa = n, \quad \text{or}$$

$$s_o \lambda_o > a_o \left[m_{\mathrm{I}} + c_x^\phi (a_x / \lambda_{\mathrm{II}}) m_{\mathrm{II}} n_{\mathrm{I}} \right] \quad \text{if} \quad \kappa < n. \blacklozenge \quad (20)$$

According to this theorem, the observer converges if the stabilizing margin $l_o = s_o \lambda_o$ is made larger than the instability margin $a_o m_{\mathrm{I}}$, which accounts for a potential self-destabilization of the observable error dynamics (Eq. 12c). The detector converges if l_o is made larger than the two-term margin $a_o m_{\mathrm{I}} + a_o c_x^\phi (a_x / \lambda_{\mathrm{II}}) m_{\mathrm{II}} n_{\mathrm{I}}$, with the second term accounting for a potential destabilization due to the coupling between the observable (12b) and the unobservable (12c) error dynamics.

Estimator Design

In this section the methodological framework that relates the solvability assessment and the construction-tuning parts of the estimator design is presented, and this includes a PI-version of the estimator. The convergence features of the estimator are examined, a pole-placement scheme for the systematic tuning of gains is introduced, and the performance-robustness compromise of the estimator is discussed.

P-estimator

In the next corollary to Theorem 1, the inequalities of the convergence of the P-estimator are presented. First, let us introduce the inequality

$$\| e^{tA(s_o)} \| \le A_a(s_o) e^{-tL_a(s_o)}, \qquad 0 < s_o < \infty;$$

$$A(s_o) = \begin{bmatrix} -L_{\mathrm{I}}(s_o) & a_o M_{\mathrm{II}} \\ A_{\mathrm{II}} N_{\mathrm{I}} & -L_{\mathrm{II}} \end{bmatrix}, \qquad L_{\mathrm{I}} = s_o \lambda_o - a_o M_{\mathrm{I}} \quad (21)$$

$$A_a(s_o) > 1, \qquad 0 < L_a(s_o) < L_{\mathrm{II}}, \qquad \lim_{s_o \to \infty} [A_a(s_o), L_a(s_o)] = (1, L_{\mathrm{II}})$$

associated to the stability of matrix A (i.e., the fulfillment of inequality 20 of Theorem 1 with $\kappa < n$).

Corollary 1 (Alvarez, 1999). Let the motion $x(t)$ of the plant (Eq. 1) be RE-estimable, let the conditions of Theorem 1 be met, and let the parameters s_u and s_o be chosen so that

Table 1. Parameters of the Estimator RE-Convergence

	Observer and Detector	$a_{xu} = F_u \sigma_{uo}$		$\sigma_o = a_o(D_x \Vert \chi_o - x_o \Vert + D_u \Vert \chi_{uo} - x_{uo} \Vert + D_r \epsilon_r)$	
	Observer	Detector		Observer	Detector
b_y	$(a_o/L_I)(M_u b_u + M_r \epsilon_r)$	$(a_o/L_I)(M_u b_u + M_{II} b_a)$	b_x^{**}	$F_r \epsilon_r$	$[(\mu_r/L_{II})F_{zII} + F_r]\epsilon_r$
b_x	$F_z b_y + F_u b_u + F_r \epsilon_r$	$F_{zI} b_y + F_{zII} b_a + F_u b_u - F_r \epsilon_r$	$\mathbf{a_v}$	$\sigma_o + a_o M_u \sigma_{uo}/(l_u - L_I)$	$\sigma_{Io} + a_o M_u \sigma_{uo}/(l_u - L_I)$
b_y^*	$(a_o/L_I) M_r \epsilon_r$	$(a_o/L_I) M_{II} b_a^*$	$\mathbf{a_x}$	$F_z \mathbf{a_v}$	$F_{zI} \mathbf{a_v}$
b_x^*	$F_z b_y^* + F_r \epsilon_r$	$F_{zI} b_{\mathbf{v}}^* + F_{zII} b_a^* + F_r \epsilon_r$	$\mathbf{a_x^*}$	$F_z \sigma_o$	$F_{zI} \sigma_{Io}$
	Detector	$\mathbf{a_{ya}} = a_o M_{II} \mathbf{a_a}/(L_I - L_a)$		$\mathbf{a_{ya}^*} = a_o M_{II} \mathbf{a_a^*}/(L_I - L_a)$	$\mathbf{a_{xa}} = F_{zI} \mathbf{a_{ya}} + F_{zII} \mathbf{a_a}$
	$\mathbf{a_{xa}^*} = F_{zI} \mathbf{a_{ya}^*} + F_{zII} \mathbf{a_a^*}$	$\mathbf{a_{xa}^{**}} = F_{zII} \sigma_o$		$\mathbf{a_a} = A_a[\sigma_o + \mu_u \sigma_{uo}/(l_u - L_a)]$	$\mathbf{a_a^*} = A_a \sigma_o$
	$b_a = (A_a/L_a)(\mu_u b_u + \mu_r \epsilon_r)$	$b_a^* = (A_a/L_a)\mu_r \epsilon_r$		$\mu_u = \Vert (a_o M_u,\ A_{II} N_u)' \Vert$	$\mu_r = \Vert (a_o M_r,\ A_{II} N_r)' \Vert$
	$\sigma_{Io} = a_o(D_{Ix} \Vert \chi_o - x_o \Vert + D_{Iu} \Vert \chi_{uo} - x_{uo} \Vert + D_{Ir} \epsilon_r)$			$\sigma_{IIo} = A_{II}(D_{IIx} \Vert \chi_o - x_o \Vert + D_{IIu} \Vert \chi_{uo} - x_{uo} \Vert + D_{IIr} \epsilon_r)$	

Note: A boldface letter has dependency on s_u and/or s_o.

the following inequality is met (in this Corollary and in Table 1, a boldface letter has dependency on s_u and/or s_o)

$$l_u = s_u \lambda_u > \mathbf{L_I} = s_o \lambda_o - a_o \mathbf{M_I} \quad \text{if} \quad \kappa = n, \quad \text{or}$$
$$l_u > \mathbf{L_I} > L_{II} \quad \text{if} \quad \kappa < n,$$

meaning that the exo-observer error dynamics (Eq. 19a) are faster than the observable error dynamics (Eq. 12b), which in turn are faster than the unobservable error dynamics (Eq. 12c). Then

(i) The exo-observer (Eq. 19a) RE-converges as

$$\Vert \chi_u(t) - x_u(t) \Vert \le \sigma_{uo}\, e^{-l_u(t-t_o)} + b_u;$$
$$\sigma_{uo} = a_u \Vert \chi_{uo} - x_{uo} \Vert, \qquad b_u = (a_u/l_u)\epsilon_v;$$

As $s_u \to \infty$: $\chi_u(t) = x_u(t)$.

(ii) The observer (Eq. 19 with $\kappa = n$) RE-converges as

$$\Vert \psi(t) - y(t) \Vert \le \mathbf{a_y}\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{b_y},$$
$$\Vert \chi(t) - x(t) \Vert \le \mathbf{a_x}\, e^{-\mathbf{L_I}(t-t_o)} + a_{xu}\, e^{-l_u(t-t_o)} + \mathbf{b_x}$$

As $s_u \to \infty$: $\Vert \psi(t) - y(t) \Vert \le \sigma_o\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{b_y^*}$,

$$\Vert \chi(t) - x(t) \Vert \le \mathbf{a_x^*}\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{b_x^*}$$

As s_u, $s_o \to \infty$: $\psi(t) = y(t)$,

$$\Vert \chi(t) - x(t) \Vert \le b_x^{**}.$$

(iii) The detector (Eq. 19 with $\kappa < n$) RE-converges as

$$\Vert \psi(t) - y(t) \Vert \le \mathbf{a_y}\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{a_{ya}}\, e^{-\mathbf{L_a}(t-t_o)} + \mathbf{b_y}$$
$$\Vert \chi(t) - x(t) \Vert \le \mathbf{a_x}\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{a_{xa}}\, e^{-\mathbf{L_a}(t-t_o)} + a_{xu}\, e^{-l_u(t-t_o)} \sigma_{uo} + \mathbf{b_x}$$

As $s_u \to \infty$: $\Vert \psi(t) - y(t) \Vert \le \sigma_{Io}\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{b_y^*}$,

$$\Vert \chi(t) - x(t) \Vert \le F_{zI} \sigma_{Io}\, e^{-\mathbf{L_I}(t-t_o)} + \mathbf{a_{xa}^*}\, e^{-\mathbf{L_a}(t-t_o)} + \mathbf{b_x^*}$$

As s_u, $s_o \to \infty$: $\psi(t) = y(t)$,

$$\Vert \chi(t) - x(t) \Vert \le \mathbf{a_{xa}^{**}}\, e^{-L_{II}(t-t_o)} + b_x^{**}.$$ ♦

From this corollary, the following convergence features are drawn. In the estimator case, by tuning the parameters s_u and s_o sufficiently large: (i) the output and the state can converge arbitrarily fast; (ii) the output offset can be made arbitrarily small; and (iii) the size of the state offset can be made arbitrarily close to its limiting value b_x^{**}. In the detector case, by tuning the parameters s_u and s_o sufficiently large, (i) the output can converge arbitrarily fast; (ii) the output offset can be made arbitrarily small; (iii) the state can converge with a speed (L_a) arbitrarily close to the one (L_{II}) of the unobservable error motion; and (iv) the size of the state offset can be made arbitrarily close to its limiting value b_x^{**}. These convergence properties identify the basic capabilities and limitations of the estimator performance. In an implementation, these capabilities will be limited by the presence of measurement noise and of numerical errors, and their handling will be a central issue in the tuning scheme to be presented later.

PI-estimator

In order to have the possibility of improving the output matching and offset reduction capabilities, a PI version of the estimator is presented in this section. The idea is to modify the P-estimator to compensate for the persistent disturbance caused by the model parameter error e_r.

Since the exo-observable (e_u in Eq. 12a) and observable (e_I in Eq. 12b) error motions can be made sufficiently faster than the unobservable (e_{II} in Eq. 12c) error motion, the disturbance q_I of the observable error dynamics (Eq. 12b) can be written as follows (q_s and q_f are defined in Appendix A)

$$q_I(e_I, e_{II}, e_u, e_r, t) = q_f(e_I, e_u, t) + q_s(e_{II}, e_r, t),$$
$$q_f(0, 0, t) = q_s(0, 0, t) = 0, \quad (22)$$

where q_f is a fast vanishing disturbance, and q_s is a slow persistent disturbance that can be regarded as an additional state x_q for which a fast estimate χ_q can be obtained from a battery of integrators (one for each output)

$$\dot{\chi}_q = K_I(s_o)[y - h(\chi, \rho)], \ \chi_{q(t_0)} = 0;$$
$$K_I(s_o) = \text{diag}\left(s_o^{\kappa_1+1} k_1^I, \ldots, s_o^{\kappa_m+1} k_m^I\right), \quad (23)$$

provided the gain pair $[(K_o(s_o), K_I(s_o)]$ is appropriately tuned and the compensation state χ_q is adequately incorporated into the P-estimator.

The construction of the PI-estimator and its convergence criterion are presented in the next theorem. First, let us require the entries of the reference gain pair $[K_o(1), K_I(1)]$ to set stable the (augmented) reference LNPA output error dynamics

$$\mathbf{v}_i^{(\kappa_i+1)} + k_{1i}^o \mathbf{v}_i^{(\kappa_i)} + \cdots + k_{\kappa_i i}^o \mathbf{v}_i^{(1)} + k_i^I \mathbf{v}_i = 0,$$
$$\mathbf{v}_i = \psi_i - y_i; \qquad 1 \le i \le m, \quad (24)$$

so that the parametrized matrix $A_o^e(s_o)$ (defined in Appendix A) of the quasi-linear estimation error dynamics (Eq. 28) meets the E-stability inequality

$$\| e^{tA_o^e(s_o)} \| \le a_o^e \, e^{-s_o \lambda_o^e t}, \quad (25)$$

where the pair (a_o^e, λ_o^e) is set by the reference gain pair $[K_o(1), K_I(1)]$, and is independent of s_o.

Theorem 2 (Proof in Appendix B). Let the motion $x(t)$ of the plant (Eq. 1) be RE-estimable, let the gains $K_u(s_u)$ (Eq. 13a) and $G(\chi, \chi_u, \rho)$ (Eqs. 19c and 13b) be in the form of the P-estimator (Eq. 19), the I-gain $K_I(s_o)$ be given by Eq. 23, and let the entries of $K_u(1)$ and $[K_o(1), K_I(1)]$ set stable the reference LNPA output error dynamics 14a and 24, respectively. Then, the PI-estimator

$$\dot{\chi}_u = \Gamma_u \chi_u + K_u(s_u)(u - \Delta_u \chi_u), \qquad G_I(\chi, \chi_u, \rho)$$
$$= \Theta_I(\chi, \chi_u)\Pi_o K_I(s_o) \qquad \psi_u = \Delta_u \chi_u \quad (26a)$$
$$\dot{\chi} = f(\chi, \Delta_u \chi_u, \rho) + G(\chi, \chi_u, \rho)[y - h(\chi, \rho)]$$
$$+ G_I(\chi, \chi_u, \rho) \int_{t_o}^{t} [y - h(\chi, \rho)] \, d\tau, \qquad \psi = h(\chi, \rho) \quad (26b)$$

yields a RE-convergent estimate $\chi(t)$ of $x(t)$ if the parameter s_o is chosen sufficiently large so that the following inequality is met:

$$s_o \lambda_o^e > a_o^e m_I \text{ if } \kappa = n, \qquad \text{or}$$
$$s_o \lambda_o^e > a_o^e [m_I + c_x^\phi (a_x/\lambda_{II}) m_{II} n_I] \qquad \text{if} \quad \kappa < n, \quad (27)$$

where $\{m_I, m_{II}, n_I, a_x/\lambda_{II}$, and $c_x^\phi\}$ is defined in Theorem 1, and (a_o^e, λ_o^e) in Eq. 25. ◆

From the proof (in Appendix B) of the preceding theorem, in *e*-coordinates (Eq. 10), the estimation error dynamics of the PI-estimator (Eq. 26) are given by (the matrices A_o^e, Π_o^e and Δ_o^e, and T, and the vector e_q are defined in Appendix A),

$$\dot{e}_u = A_u e_u - \Pi_u v(t), \qquad \mu = \Delta_u e_u \quad (28a)$$
$$\dot{e}_e = A_o^e e_e + \Pi_o^e q_I[e, e_u, v(t), e_r, t], \qquad \mathbf{v} = \Delta_o^e e_e \quad (28b)$$
$$\dot{e}_{II} = \omega(e_{II}, t) + q_{II}[e, e_u, v(t), e_r, t], \quad e_e' = T[e_I', e_q']' \quad . \quad (28c)$$

The interpretation of the attainment of RE-convergence with the fulfillment of the inequality (Eq. 27) of the last theorem is similar to the one given (after Theorem 1) for the P-estimator case.

In the corollary to Theorem 2, the inequalities of the RE-convergence of the PI-estimator are presented. First, let us introduce the inequality (a_o^e and λ_o^e are defined in Eq. 27)

$$\| e^{tA_e(s_o)} \| \le [A_a^e(s_o)] \, e^{-tL_a^e(s_o)}, \qquad 0 < s_o < \infty;$$
$$A_e(s_o) = \begin{bmatrix} -L_I^e(s_o) & a_o^e M_{II} \\ A_{II} N_I & -L_{II} \end{bmatrix}, \qquad L_I^e = s_o \lambda_o^e - a_o^e M_I \quad (29)$$
$$A_a^e(s_o) > 1, \qquad 0 < L_a^e(s_o) < L_{II}$$
$$\lim_{s_o \to \infty} [A_a^e(s_o), L_a^e(s_o)] = (1, L_{II})$$

associated to the stability of the matrix A_e, or equivalently, to the fulfillment of the inequality (Eq. 27) of Theorem 2 with $\kappa < n$.

Corollary 2 (proof in Appendix B). Let the motion $x(t)$ of the plant (Eq. 1) be RE-estimable, let the conditions of Theorem 1 be met, and let the parameters s_u and s_o be chosen so that (in this corollary and in Table 1, a boldface letter has dependency on s_u and/or s_o)

$$l_u = s_u \lambda_u > L_{\mathbf{I}}^e = s_o \lambda_o^e - a_o^e M_I \qquad (\text{if } \kappa = n),$$
$$\text{or} \qquad l_u > L_{\mathbf{I}}^e > L_{II} \qquad (\text{if } \kappa < n),$$

meaning that the exo-observer error dynamics (Eq. 28a) are faster than the observable error dynamics (Eq. 28b), which in turn are faster than the unobservable error dynamics (Eq. 28c). Then, the state and output estimates of the PI-estimator (Eq. 26) RE-converge with the inequalities of Corollary 1 and Table 1, with $\{(a_o, \lambda_o)$ (Eq. 15b), (A_a, L_a) (Eq. 21)$\}$ replaced with $\{(a_o^e, \lambda_o^e)$ (Eq. 25), (A_a^e, L_a^e) (Eq. 29)$\}$.

The interpretation of the RE-convergence features of the PI-estimator are similar to the ones that were drawn (after Corollary 1) for the P-estimator. Comparing with the P-estimator and using the same tuning scheme (that will be presented in the next section), one sees that $a_o^e > a_o$, $A_a^e > A_a$, $L_I^e < L_{\mathbf{I}}$, and that $L_a^e < L_a$, in Corollaries 1 and 2. This means that the PI-design yields smaller output and state offsets at the cost of slower and more oscillatory convergence. As is done in the design of linear controllers, the engineer must evaluate whether integral action is appropriate, depending on the particular plant and on its estimation requirements. This will be illustrated below in the application example.

Exo-observer tuning

Since the handling of noise in the measured inputs is the central point of the exo-observer design, its gains can be tuned with the standard linear optimal stochastic filtering techniques. First let v_i and w_i be zero-mean, uncorrelated white model, and measurement noises with intensities q_i and r_i, respectively; then write the stochastic version of the exosystem (Eq. 7a) (Γ_i^u, π_i^u, and δ_i^u are defined in Appendix A)

$$\dot{x}_i^u = \Gamma_i^u x_i^u + \pi_i^u v_i(t), \qquad u_i = \delta_i^u x_i^u + w_i(t), \qquad 1 \le i \le p$$

Table 2. Reference Gains

(a) Exo-Observer ($\omega = \omega_i^u$) $k_{1i}^u, \ldots, k_{\nu_i}^u$	(b) Plant Observer ($\omega = \omega_i^o$, $\xi = \xi_i^o$) $k_{1i}^o, \ldots, k_{\kappa_i i}^o$ (P-est.); or $k_{1i}^o, \ldots, k_{\kappa_i i}^o, k_i^{\mathrm{I}}$ (PI-est.)
ω	ω
$1.4\omega,\ \omega^2$	$2\xi\omega,\ \omega^2$
$2\omega, 2\omega^2,\ \omega^3$	$(2\xi+1)\omega, (2\xi+1)\omega^2,\ \omega^3$
$2.6\omega, 3.4\omega^2, 2.6\omega^3,\ \omega^4$	$4\xi\omega, (4\xi^2+2)\omega^2, 4\xi\omega^3,\ \omega^4$
$3.24\omega, 5.24\omega^2, 5.24\omega^3, 3.24\omega^4,\ \omega^5$	$(4\xi+1)\omega, (4\xi^2+4\xi+2)\omega^2, (4\xi^2+4\xi+2)\omega^3, (4\xi+1)\omega^4,\ \omega^5$

and recall its optimal steady-state filter (Kwakernaak and Sivan, 1972)

$$\dot{\chi}_i^u = \Gamma_i^u \chi_i^u + \pi_i^u \upsilon_i(t) + k_i^u(u_i - \delta_i^u \chi_i^u), \qquad k_i^u = r_i^{-1}\Sigma_i \delta_i^{u'}, \qquad 1 \le i \le p,$$

where the $(\nu_i x \nu_i)$-matrix Σ_i is given by the solution of the Riccati equation

$$\Sigma_i \Gamma_i^u + \Gamma_i^{u'} \Sigma_i + q_i \pi_i^u \pi_i^{u'} - r_i^{-1} \Sigma_i \delta_i^{u'} \delta_i^u \Sigma_i = 0, \qquad 1 \le i \le p.$$

Fix a reference model-to-measurement noise quotient (q_i^r/r_i^r), and solve for k_i^u in terms of ω_i^u and s_o, which are defined as follows

$$\omega_i^u = (q_i^r/r_i^r)^{1/(2\upsilon_i)}, \qquad s_u = \left[(q_i/r_i)^{1/(2\upsilon_i)}\right]\omega_i^u, \qquad 1 \le i \le p,$$

so that the optimal gain $k_i^o(s_o)$ is in the parametrized form of the ith vector entry of the block-diagonal gain matrix $K_u(s_u)$ (Eq. 13a), with its reference gain $k_i^u(1)$ set by ω_i^u and given (up to exo-observability index $\upsilon_i = 5$) in Table 2a. The corresponding ith exo-observer error dynamics (Eq. 14a) have a time-scaled Butterworth's pole configuration (D'azzo and Houpis, 1981), as shown in Figure 1a: refer to ω_i^u as the reference characteristic frequency, draw a circle with radius $s_o \omega_i^u$, center it at the origin of the complex plane, place $2\nu_i$ equidistant poles along the circle, and keep the stable ones. That there exists a relationship between the optimal stochastic observer and Butterworth's pole structure is a known fact in linear Kalman filtering (Kwakernaak and Sivan, 1972).

Plant observer tuning

Should the nonlinear error q_{I} in the observable error dynamics (Eq. 12b or Eq. 28b) be sufficiently small, the convergence condition (Eq. 20 or Eq. 27) would be easily met, the estimator divergence would not be a problem, and the estimator gain matrix, K_o or (K_o, K_{I}), should be tuned with the noise-oriented pole-placement approach of the last section. In principle, the same kind of obstacle may be at work in the nonlinear EKF observer, judging from the kind of tuning and divergence problems that have been reported in the literature. On the other hand, for large (say greater than two) observability indices, the noise-oriented Butterworth tuning scheme places a pole close to the imaginary axis, with an amplitude that grows with the parameter s_o, and this means propensity toward divergence or convergence with poor robustness. To confront this problem, a pole-placement approach is presented next.

Rewrite as follows the ith reference LNPA output error equation (Eq. 14b or Eq. 24)

$$\mathbf{v}_i^{(n_i)} + k_1^i \mathbf{v}_i^{(n_i-1)} + \cdots + k_{n_i}^i \mathbf{v}_i = 0,$$

$$n_i = \kappa_i(P\text{-est.}) \text{ or } \kappa_i + 1 \text{ (PI-est)}. \tag{30}$$

and require its characteristic polynomial

$$(\gamma_i)^{n_i} + k_1^i(\gamma_i)^{(n_i-1)} + \cdots + k_{n_i}^i(\gamma_i) = 0$$
$$= (\gamma_i - \gamma_1^i)(\gamma_2 - \gamma_2^i)\cdots(\gamma_i - \gamma_{n_i}^i) \tag{31}$$

to have n_i prescribed reference (i.e., with $s_o = 1$) poles $\gamma_1^i, \ldots, \gamma_{n_i}^i$, according to the following robustness-oriented criteria: (1) the condition number (i.e., the ratio of the modulus of the fastest to the slowest pole) must be one, in order to attenuate the effect of the disturbance q_{I} of the error dynamics (Eq. 12 or Eq. 28), and (2) each pole must have a sufficiently large damping factor to prevent excessively oscillatory behavior. Thus, if n_i is an even number, the reference LNPA output error dynamics (Eq. 30) must have $n_i/2$ repeated pairs of complex poles with reference characteristic frequency ω_i^o and a sufficiently large (say $\xi_i > 0.71$) damping factor; otherwise, if n_i is odd, $n_i - 1$ poles are assigned in the same way, and the n_i-th pole is set to be real with characteristic frequency ω_i^o. This is, for $s_o = 1$,

$$\gamma_{i,\,i+1}(1) = -\,\omega_i^o\left(\xi_i \pm \sqrt{\xi_i - 1}\right), \qquad i = 1, 3, \ldots, n_i - 1;$$
$$\gamma_{n_i}(1) = -\,\omega_i^o \qquad \text{if} \quad n_i \text{ is odd}.$$

The comparison of coefficients in the two-equation set 31 yields the ith reference gain vector $k_i(1)$ shown in Table 2b, up to $n_i = 5$, and the corresponding s_o-time scaled pole patterns $\{\gamma_i(s_o) = s_o \gamma_i(1),\ s_o > 0\}$ are shown in Figure 1b. In contrast to the noise-oriented Butterworth pole pattern, here the designer can avoid the location of poles near the imaginary axis, or equivalently, can prevent the estimator divergence or convergence with poor robustness. In principle, the gain parametrization (Eq. 13b, or Eqs. 13b and 23) in conjunction with information both on the disturbances (q_{I} and q_{II}) of the estimation error dynamics (Eq. 13 or Eq. 28), and on the modeling and measurement noise, can be the point of departure to study other ways for setting the reference pole pattern, say by resorting to robust filtering techniques (Vidyasagar, 1987).

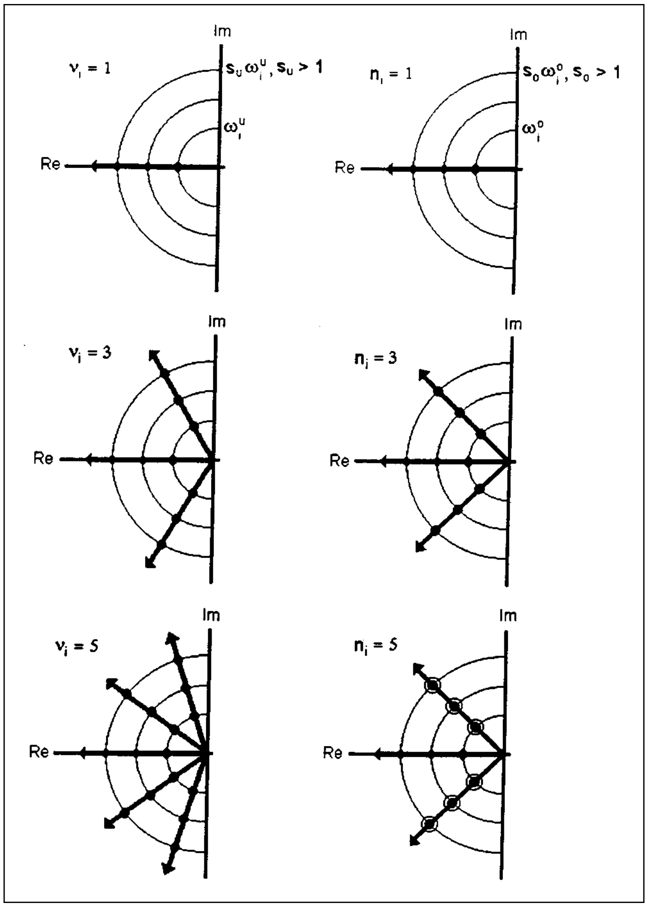

Figure 1. (a) Exo-observer and (b) plant observer pole patterns.

Performance-robustness compromise

In this section the nature of the compromise between the dynamic performance and the robustness of the proposed estimation design is discussed.

From Corollaries 1 and 2, the amplitude a_x that bounds the size of the transient part of the state error, $\chi(t)-x(t)$, is proportional to the "condition number" C_x^{ϕ} (defined in Eq. 18) of the estimability map ϕ along the motion of the plant. In the case of a detector, the resonant instability margin is proportional to C_x^{ϕ} (see Eqs. 18, 20, and 27). Therefore, a poorly conditioned map ϕ should lead to a poor estimator convergence (i.e., with small tolerance to initial-state, input, and model parameter errors), and the designer may have to consider sacrificing dynamic performance for robustness, according to the next rationale.

In order to attain the fastest rate of convergence in a nominal design (i.e., without modeling errors), the estimability property should be met with the largest possible overall observability index κ. If there are parameter errors and the plant motion is sensitive to them, the observability index κ may have to be reduced to prevent an excessive propagation of errors through high-order partial derivatives of the maps f and h in the maps ϕ and φ of the estimability property of the plant motion, provided that its unobservable motion does not become unstable or stable with poor robustness. Thus, the choice of the observability index set must regarded as a degree of freedom in the design, in a way that is analogous to the choice of the controllability index set in a geometric nonlinear control design (Padilla and Alvarez, 1997). If there are various possibilities of sensing devices (i.e., of maps h), their selection should also be a degree of freedom in the design.

Concluding remarks

Definition 1 provides a test to assess, either analytically or numerically, the estimability property of a motion or a set of motions of the plant, with the choice of the observability index set being a degree of freedom in the estimator design. Theorem 1 or 2 yield a systematic construction of the P or PI estimator, respectively; each one sets a simple and systematic tuning procedure that can be done either with the proposed pole-placement approaches or with any other technique available from the ample repertoire for designing linear single-output filters and single-input controllers. Corollaries 1 and 2 show the interplay and compromise between estimability structure, parameter gains, rate of convergence, size of the offset, size of the convergence neighborhood, the attainment of convergence, and its degree of robustness.

The convergence features (speed, amplitude, offset, and robustness) are determined by the inherent properties of the plant (i.e., of maps f and h) along its input-state motion, on the one hand, and on the other, follow from the designer's structural and constructive decisions. Two structural decisions involve choosing the measurement-device set and its observability index set, and two constructive decisions have to do with the choice of a P- or a PI-estimator and that of the reference pole patterns in the gain tuning scheme.

The RE-convergence of the proposed estimation design is local in the sense that results are valid in some neighborhood (of undefined size and shape, not necessarily small) of the plant motion. In principle, the convergence approach of the present work can be extended to the semiglobal (Isidori, 1995) case, where the estimator gains can be tuned to ensure convergence for a prescribed compact set of initial states.

Estimation of Free-Radical Homopolymer Reactors

Reactor class and its estimation problem

Consider the stirred-tank reactor depicted in Figure 2, where a strongly exothermic free-radical homopolymerization takes place, heat exchange being enabled by a heating/cooling jacket. The reactor dynamics are described by the six-state, eight input, three-output equation set:

$$\dot{I} = -r_I(I,T) + \epsilon I r_p(I,m,T) + (i_e - q_e I)/V := f_I,$$

$$u = (i_e, q_e, q, T_e, T_c, m_e, \mu_{0e}, \mu_{2e})' \quad (32a)$$

$$\dot{m} = -(1-\epsilon m) r_p(I,m,T) + q_e(m_e - m)/V := f_m,$$

$$y_1 = m \quad (32b)$$

$$\dot{T} = \beta(m) r_p(I,m,T) - \gamma(m,T,V)(T_c - T) + q_e(1-\epsilon m_e) \times (T_e - T)/[(1-\epsilon m)V] := f_T, \quad y_2 = T \quad (32c)$$

$$\dot{V} = -\epsilon V r_p(I,m,T) + q_e - q := f_V, \quad y_3 = V \quad (32d)$$

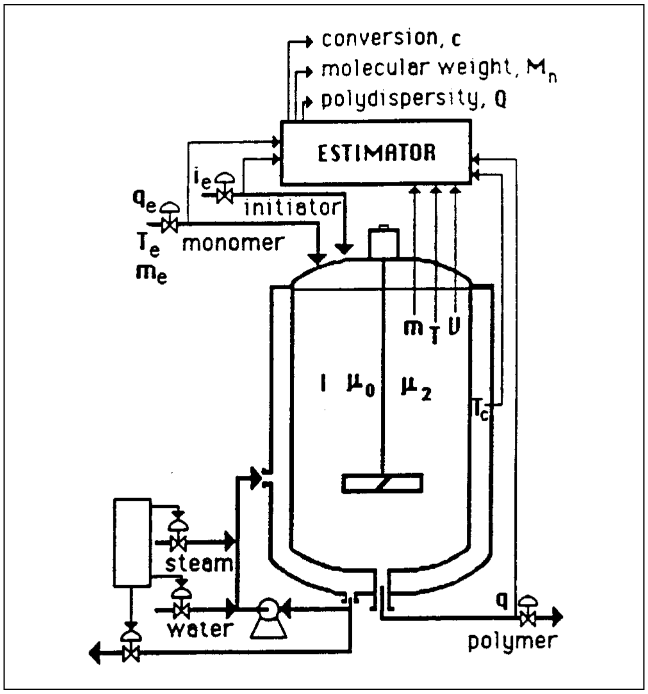

Figure 2. Polymerization reactor and its estimation scheme.

$$\dot{\mu}_0 = r_0(I,m,T) + \epsilon\mu_0 r_p(I,\ m,T) + q_e(\mu_{0e} - \mu_0)/V := f_{\mu 0} \tag{32e}$$

$$\dot{\mu}_2 = r_2(I,m,T) + \epsilon\mu_2 r_p(I,m,T) + q_e(\mu_{2e} - \mu_2)/V := f_{\mu_2} \tag{32f}$$

With the state $x = (I,\ m,\ T,\ \mu_0,\ \mu_2,\ V)'$, output (y), and input (u) vector notation, the reactor model has the estimator design form of Eq. 1.

The states of the plant are I (concentration of initiator); m (dimensionless concentration M/M^o of monomer, where M and M^o are the molar concentrations of monomer and of pure monomer), T (temperature), μ_0 [zeroth moment of the CLD (chain length distribution)], μ_2 (second moment of the CLD), and V (volume). The exogenous inputs are i_e (initiator feed rate), q_e (inlet flow rate), q (exit flow rate), T_e (inlet temperature), and T_c (coolant jacket temperature). The measured outputs are m [using a densitometer (Schuler and Papadopolou, 1986) or a refractive index sensor (Ellis et al., 1994)], temperature T (using a thermocouple), and volume V (by reactor gravimetry or using a level sensor).

The terms r_I and r_p are the rates of initiator decomposition and polymerization, respectively, and the terms r_0 and r_2 are the rates of change of the zeroth and second CLD moments, respectively. The terms β and γ are the ratios of heat generation and exchange capabilities to heat capacity, respectively. The terms r_I, r_p, r_0, r_2, β, γ are smooth and strictly positive scalar fields in the reactor state-space (for the modeling considerations see Alvarez et al., 1992 and 1994). With suitable choices of the feed and exit flow rates, the preceding model can represent batch ($q_e = q = 0$), semibatch ($q = 0$), and continuous operations ($q_e = q + \epsilon r_p V$, $q \neq 0$). Due to the presence of the gel effect (i.e., autoacceleration of the polymerization rate r_p and decrease of the heat-transfer function γ due to the increase of viscosity with the fraction of polymeric material), a continuous reactor can have multiplicity of steady states (Alvarez et al., 1990), and a batch or semibatch reactor can have an open-loop unstable-state motion (Alvarez et al., 1994).

The reactor estimation problem follows. Based on the three-measurement vector $y(t)$, obtain estimates of the conversion c, the average molecular weight M_n, and the polydispersity Q:

$$c = (1-m)/(1-\epsilon m), \qquad M_n = \rho_m (1-m)/[(1-\epsilon)\mu_o],$$
$$Q = [(1-\epsilon)/(1-m)]^2(\mu_2/\mu_0),$$

which are key variables to monitor the safety level, the production rate, and the product grade of an industrial reactor.

Solvability of the estimation problem

The assessment of the solvability of the reactor estimation problem follows from a straightforward testing of the RE-estimability condition of Definition 1, and the results are presented in the following proposition, which is a consequence of two physical properties that are met by any free-radical homopolymer reactor: (1) the polymerization rate r_p is a strictly positive, L-continuous function that increases monotonically (i.e., $\partial r_p/\partial x_1 > 0$) with the concentration of initiator, and (2) the monomer dynamics with gel effect is the sole source of reactor motion instability.

Proposition 1 (Proof in Appendix C). In the class of free-radical homopolymer reactors (Eq. 32):

(i) The motions are RE-detectable with the following observability index sets

$$\mathscr{k}_1 = \{1,1,1\}, \qquad \mathscr{k}_2 = \{2,1,1\}, \qquad \mathscr{k}_3 = \{1,2,1\}, \qquad \mathscr{k}_4 = \{1,1,2\}$$

(ii) For the case with $\mathscr{k}_1$, $\phi_{\rm I} = (m,\ T,\ V)'$, $\phi_{\rm II} = (I,\ \mu_0,\ \mu_2)'$, and the unobservable dynamics are

$$[\dot{I}^*,\ \dot{\mu}_0^*,\ \dot{\mu}_2^*]' = [f_I,\ f_{\mu_0},\ f_{\mu_2}]'_{[I^*,\ m(t),\ T(t),\ V(t),\ \mu_0^*(t),\ \mu_2^*(t),\ i_e(t),\ \mu_{0e}(t),\ \mu_{2e}(t),\ q_e(t)]}$$

(iii) For the cases with $\mathscr{k}_2$, $\mathscr{k}_3$, and $\mathscr{k}_4$, $\phi_{\rm II} = (\mu_0,\ \mu_2)'$,

$$\phi_{\rm I} = (m,\ f_m,\ T,\ V)' \ \text{for}\ \mathscr{k}_2, \qquad (m,\ T,\ f_T,\ V)' \ \text{for}\ \mathscr{k}_3, \qquad (m,\ T,\ V,\ f_V)' \ \text{for}\ \mathscr{k}_4$$

and the unobservable dynamics are

$$[\dot{\mu}_0^*,\ \dot{\mu}_2^*]' = [f_{\mu_0},\ f_{\mu_2}]'_{[I(t),\ m(t),\ T(t),\ V(t),\ \mu_0^*(t),\ \mu_2^*(t),\ \mu_{0e}(t),\ \mu_{2e}(t),\ q_e(t)]}. \quad \blacklozenge$$

According to this proposition, the cases with $\mathscr{k}_2$, $\mathscr{k}_3$, and $\mathscr{k}_4$ have the same RE-estimability structure, in different $\phi_{\rm I}$-

coordinates. Cases $\mathscr{k}_3$ and d_4 correspond to the so-called (laboratory or industrial scale) "calorimetric" (Varela de la Rosa et al., 1996), and (laboratory-scale) "volumetric" (Balke and Hamielec, 1973) methods to estimate the polymerization rate in a reactor, respectively. However, in an industrial reactor the volumetric method (i.e., with $\mathscr{k}_4$) would not be appropriate because of the insufficient precision of gravimetric or level standard industrial sensors.

Estimator construction and tuning

Having assessed the solvability of the reactor estimation problem, the estimator construction becomes a straightforward application of Theorem 1 (P-estimator) or 2 (PI-estimator), and the setting of the gain tuning scheme amounts to choosing the reference frequencies and the damping factors that set the reference gains $K_u(1)$ and $K_o(1)$ (P-est.) or $[K_o(1), K_I(1)]$ (PI-est.). For the gain $K_o(1)$ or $[K_o(1), K_I(1)]$, three output reference characteristic frequencies and their damping factors must be chosen

$$(\omega_1^o, \omega_2^o, \omega_3^o) = (\omega_m, \omega_T, \omega_V); \quad \text{for} \quad n_i \geq 2(\xi_1^o, \xi_2^o, \xi_3^o) = (\xi_m, \xi_T, \xi_V).$$

In the case with observability index set $\mathscr{k}_1$, the nonlinear gain G does not depend on the input $u(t)$, and this means that the measured inputs can be fed directly to the map $f(\chi, u, \rho)$ of the estimator. The gain G depends on the estimates χ_u of $u = (m_e, q_e)'$ for $\mathscr{k}_2$, $(m_e, q_e, T_e, T_c)'$ for $\mathscr{k}_3$, and $(q_e, q)'$ for $\mathscr{k}_4$, and therefore the corresponding exo-observers consist of first-order independent filters, one for each measured input. As is usually done in control practice, the reactor estimator should be driven by filtered inputs with time-scaled periods $1/(s_u \omega_i^u)$ set (say 10 to 20 times faster than the dominant period of the ith output) to track the frequency band of the exogenous inputs that affects most the reactor dynamics.

Test motion

Let us consider the polymerization of methylmethacrylate with AIBN initiator, in a continuous reactor that holds a nominal volume $\overline{V}_e$ of 2000 L and has the following nominal inputs: $\overline{q}_e = 40$ L/min of pure monomer ($\overline{m}_e = 1$, $\mu_{0e} = \mu_{2e} = 0$) at $\overline{T}_e = 300$ K are processed, the coolant temperature $\overline{T}_c$ is 300 K, the initiator feedrate $\bar{i}_e$ is 0.08 gmol/min, and the exit flow rate is $\overline{q}(t) = 34.9359$ L/min. The reactor residence time is about 50 min, meaning an unobservable motion with a settling time of at least 200 min. The model functions and parameters of this polymer reactor are given in Alvarez et al. (1992, 1994). The reactor has (at least) three steady states (Alvarez et al., 1994), which are shown in Table 3. Initially, the reactor is at values of I, m, T, μ_o, and μ_2, which correspond to the unstable steady state, but with a volume $V_o =$ 1500 L, which is 500 L below its nominal value of 2000 L. At the initial time $t_o = 0$, the reactor is subjected to a time-varying feed temperature and exit flow rate

$$T_e(t) = 300 + 10\, e^{-4t/120} \sin(2\pi t/60),$$

$$q(t) = \overline{q}_e - \epsilon V r_p(I,m,T) - (500)(4/125)\, e^{-4t/125},$$

Table 3. Reactor Steady-States and Estimator Initial State

State	Stable (Extinction)	Unstable (Saddle)	Stable (Ignition)	Estimator Initial State
I (mol/L)	2.015×10^{-3}	1.839×10^{-3}	3.2408×10^{-4}	1.5×10^{-3}
m	0.9933	0.5809	0.4331	0.6
T (K)	314.6	349.6	377.1	340.0
μ_o (mol/L)	3.6888×10^{-6}	5.2268×10^{-4}	2.3990×10^{-3}	4.0×10^{-4}
μ_2 (mol/L)	3.4940×10^{3}	9.6540×10^{4}	3.8496×10^{4}	1.05×10^{5}
V (L)	2000.0	2000.0	2000.0	1550.0
c	8.9937×10^{-3}	0.4926	0.6379	0.4729
M_n (g/mol)	2.1788×10^{6}	9.6212×10^{5}	2.8357×10^{5}	1.2×10^{6}
Q	2.0	2.0	2.0	1.827

so that, in a (2%)-settling time of 125 min, the two exogenous inputs reach their nominal values. The term $-\epsilon V r_p$ of the exit flow-rate expression does not modify the reactor estimability structure, it has been included to force the volume to reach exactly its nominal value, thus enabling a comparison with the steady states reported in Table 3. The evolution of the reactor is presented in Figure 3, which shows that the reactor dynamics are thoroughly excited, due to the competing tendencies between extinction and ignition that undergo considerable and abrupt changes. After passing through the difficult (i.e., with high conversion and temperature, strong gel effect, and limited heat removal) region of its state space, the reator reaches asymptotically its ignition (i.e., high conversion) steady state. In light of this, the proposed estimator design will be subjected to a severe test. The initiator (I), monomer (m, or conversion c), temperature (T), and moleculare weight (M_n) have settling times of ≈ 220 min (i.e., about the residence-time settling time), and the polydispersity settling time is of ≈ 300 min, implying that the settling time of the moment μ_2 and of the unobservable dynamics are of about 300 min, and this is consistent with the fact that μ_2 follows the dynamics of two "capacitors" (each one with a settling time of ≈ 200 min) in cascade interconnection.

For the robustness test, the estimator will be implemented with the following parameter errors: E_p/R (E_p: activation energy of the propagation step) is 2,250 instead of 2,190.74 cal, a_h (dimensionless proportionality constant of the heat-exchange function) is 0.67 instead of 0.74, and f_I (efficiency factor in the generation of free radicals by the initiator decomposition) is 0.55 instead of 0.58. These parameter errors signify an $\approx 16\%$ underestimation of the rate of the heat-producing propagation reaction, an $\approx 10\%$ underestimation in the capability heat removal, and a 5% underestimation of the initiator efficiency. Figure 3 shows the evolution of the reactor model with the deviated initial-state given in Table 3 and the just-mentioned parameter errors: instead of reaching the ignition steady state with a damped oscillatory motion, the model motion reaches the extinction (i.e., almost no conversion) steady state with underdamped (i.e., monotonic) responses. This divergent motion must be seen as the zero-gain case of the estimator design, and shows that the nominally stable test motion is not robust with respect to the aforementioned model parameter errors.

Reference gains

From previous dynamics and control studies (Alvarez et al., 1990, 1994) in the same reactor, we know that, at $\overline{T}$ and $\overline{V}$,

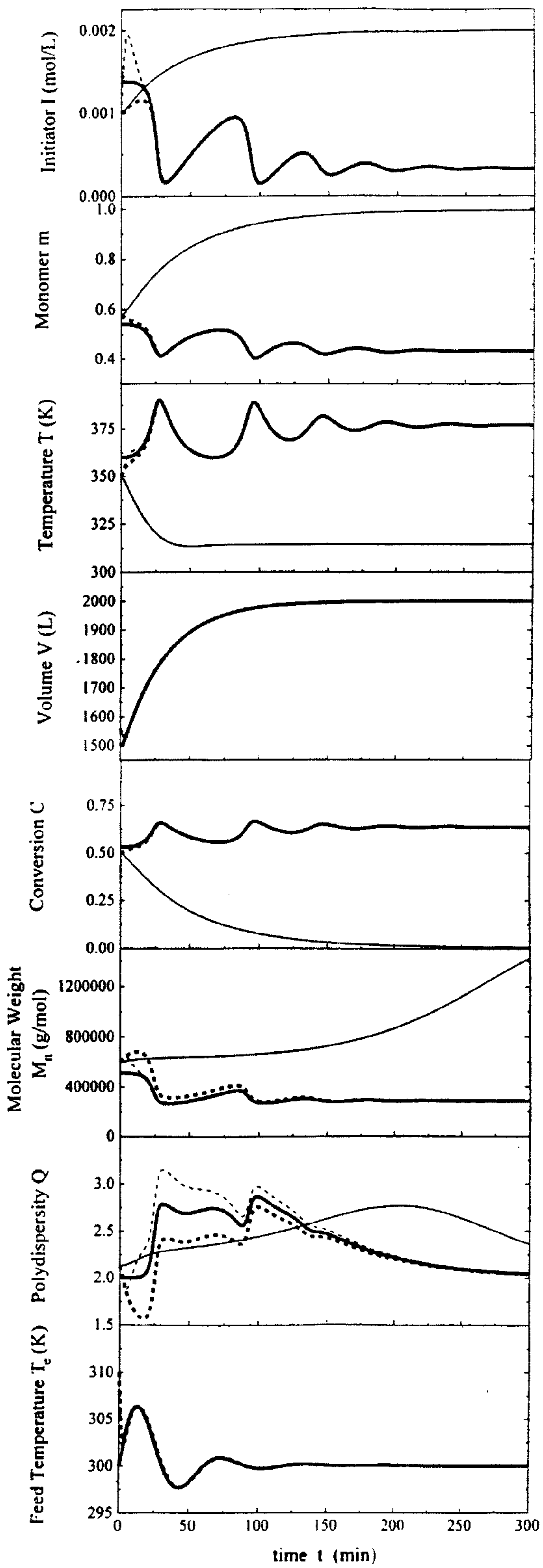

Figure 3. Evolutions of the reactor (——); of the reactor with initial-state and model parameter errors (——); and of the nominal P-estimators for Cases 1 ($\kappa = 3$:---) and 2 ($\kappa = 4$:---).

the settling time of the monomer dynamics is ≈ 125 min; and that, at $\bar{I}$, $\bar{m}$, and $\bar{V}$, the settling time of the temperature dynamics is ≈ 75 min. In order to filter the noise of the feed temperature, while keeping track of the significant period band (≈ 0 to 50/10 min) that affects the reactor dynamics, a time-scaled settling time of 3 min was chosen for the exo-observer design. Thus, the reference frequencies and damping factors for the P- or PI-estimator are set as follows

$$(\omega_m, \omega_T, \omega_V; s_u \omega_{Te}) = 4(1/125, 1/75, 1/5; 1/3)\ \text{min}^{-1},$$

$$\xi_{m/T/V} = 0.71.$$

Nominal estimation

Let us refer to the estimator design with observability index sets $k_1 = \{1, 1, 1\}$, $k_2 = \{2, 1, 1\}$, and $k_3 = \{1, 2, 1\}$ as Cases 1, 2, and 3, respectively, and let us set the time-scaling parameter $s_o = 10$, in accordance with the process-control heuristics that "the estimator must be set ten times faster than the process." The nominal (i.e., without modeling error) P-estimator was implemented, finding adequate convergent responses in the three cases, and similar responses in Cases 2 and 3. The parameter s_o was varied, finding that the estimators converged for values of s_o from 3 to 30, and that $s_o = 10$ yields an adequate functioning. The functioning of the nominal P-estimator is shown in Figure 4a, for Cases 1 and 2. As can be seen in the figure, the nominal P-estimators converge with the features of Corollary 1, with settling times that resemble closely the ones of the time-scaled reference LNPA output error dynamics: there are no offsets, the settling time (≈ 20 min.) of the observable set, $\{I, c, T\}$ for Case 1 or $(c, T\}$ for Case 2, resemble the dominant (i.e., the slowest) design settling time $\tau_m/s_o = 12.5$ min (of the monomer dynamics), and the settling time (≈ 200 min) of the polydispersity Q coincides with the one of the unobservable error dynamics. In Case 2, the error settling time (≈ 20 min) of molecular weight M_n is faster than the one (≈ 100 min) of Case 1, the reason being that the unobservable dynamics of Case 1 contain the initiator dynamics, while the unobservable dynamics of Case 2 does not.

Estimation with parameter errors

Figure 4a shows the functioning of the P- and PI-estimators for Case 1. As can be seen in the figure, the settling times of the error responses are similar to the ones of the nominal P-estimator of Case 1 in Figure 3; the P-estimator produces small output (m, T) and conversion (c) offsets, some molecular-weight (M_n) offset, and a large polydispersity (Q) offset; the PI-estimator does not have output (m, T) and conversion (c) offsets; and the M_n and Q offsets are similar to the ones of the P-case.

Figure 4b shows the functioning of the P- and PI-estimators for Case 2. The error settling times are similar to the ones of the nominal P-design in Figure 3, the P-estimator yields imperceptible output (m, T) and conversion (c) offsets, the PI-estimator yields no output (m, T) and conversion (c) offsets, the P- and PI-estimators yield offsets for M_n that are similar to the ones of Case 1 in Figure 4a. Compared

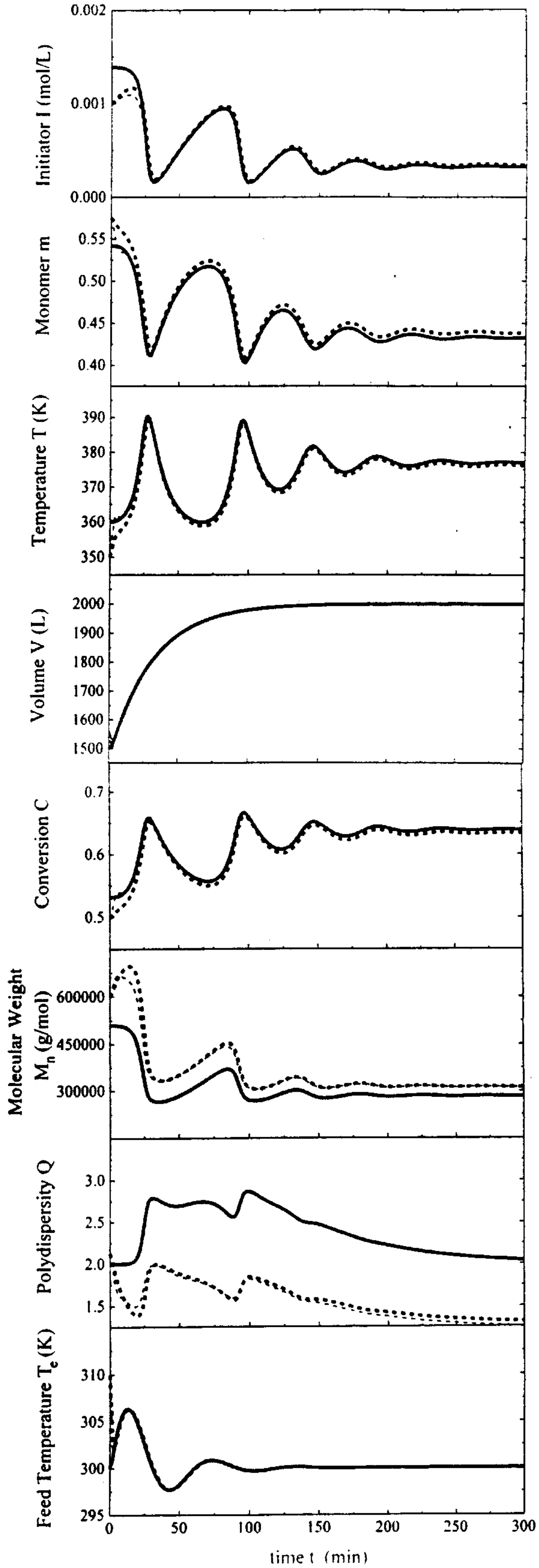

Figure 4a. Evolutions of the reactor (——) and *P* (---) and *PI* (---) estimators for Case 1 ($\kappa = 3$) with model parameter errors.

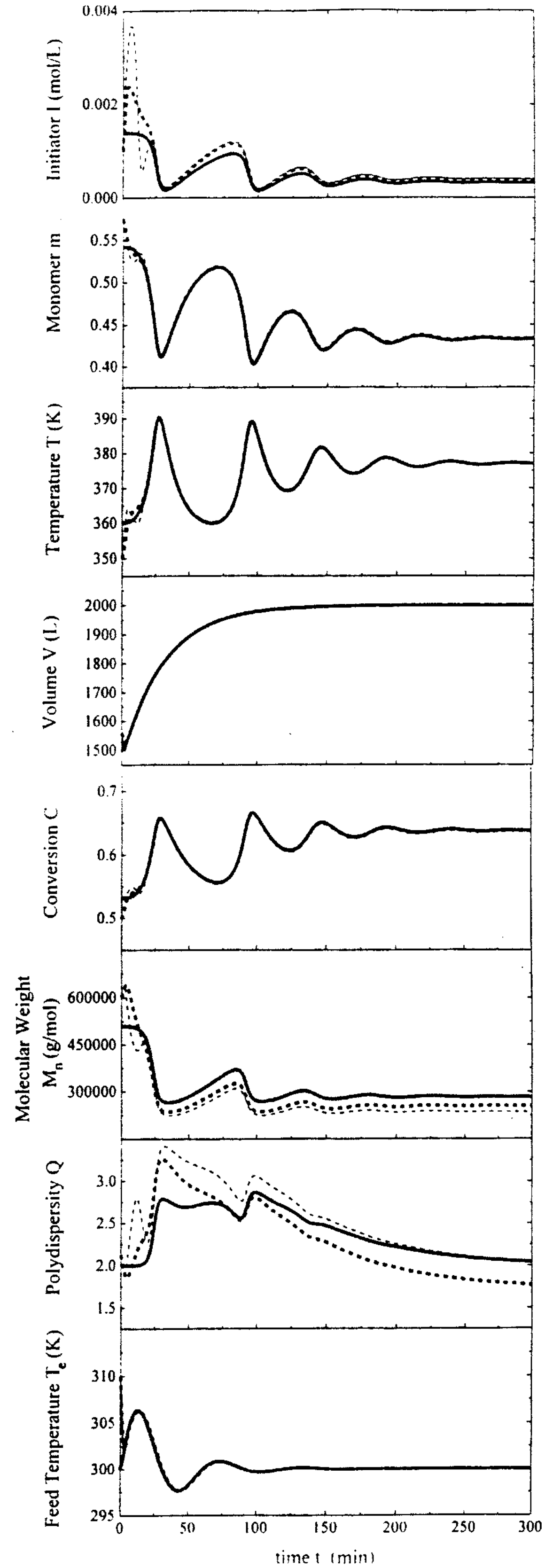

Figure 4b. Evolutions of the reactor (——) and *P* (---) and *PI* (---) estimators for Case 2 ($\kappa = 4$) with model parameter errors.

with Case 1 in Figure 4a, the P-estimator reduces the Q offset by 50%, and the PI-estimator eliminates the offset.

In this particular reactor, Case 2 (with $\kappa = 4$) performed better than Case 1 (with $\kappa = 3$), or equivalently, the case with larger overall observability index κ performed better. An example of the opposite relation between performance and the overall observability index κ can be seen in Lopez and Alvarez's 1997 estimation study for a copolymer reactor.

Estimation with measurement noise

In this section the PI-estimators of Cases 1 and 2 are tested with the zero-mean noisy measurements in Figure 5a for m (monomer), T (temperature), V (volume), and T_e (feed temperature). The noises were injected at time intervals of one minute, using Gaussian random variables with the following standard deviations (Van Dooting et al., 1992): 0.015 for monomer concentration m, 3 K for the feed and reactor temperatures, and 25 L for the volume. The functioning of the PI-estimators is shown in Figure 5b, for Cases 1 and 2. Both estimators can handle the noise well, with motion means that basically coincide with the ones of the noiseless cases of Figures 4a and 4b, and with reasonable standard deviations in the conversion, the molecular weight, and the polydispersity.

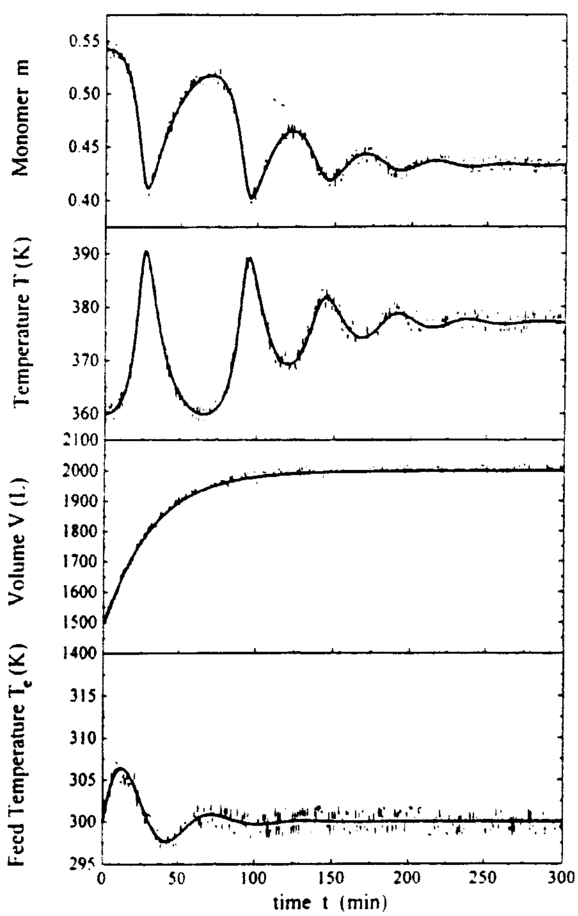

Figure 5a. Reactor outputs and inputs (——) and their noisy measurements (——).

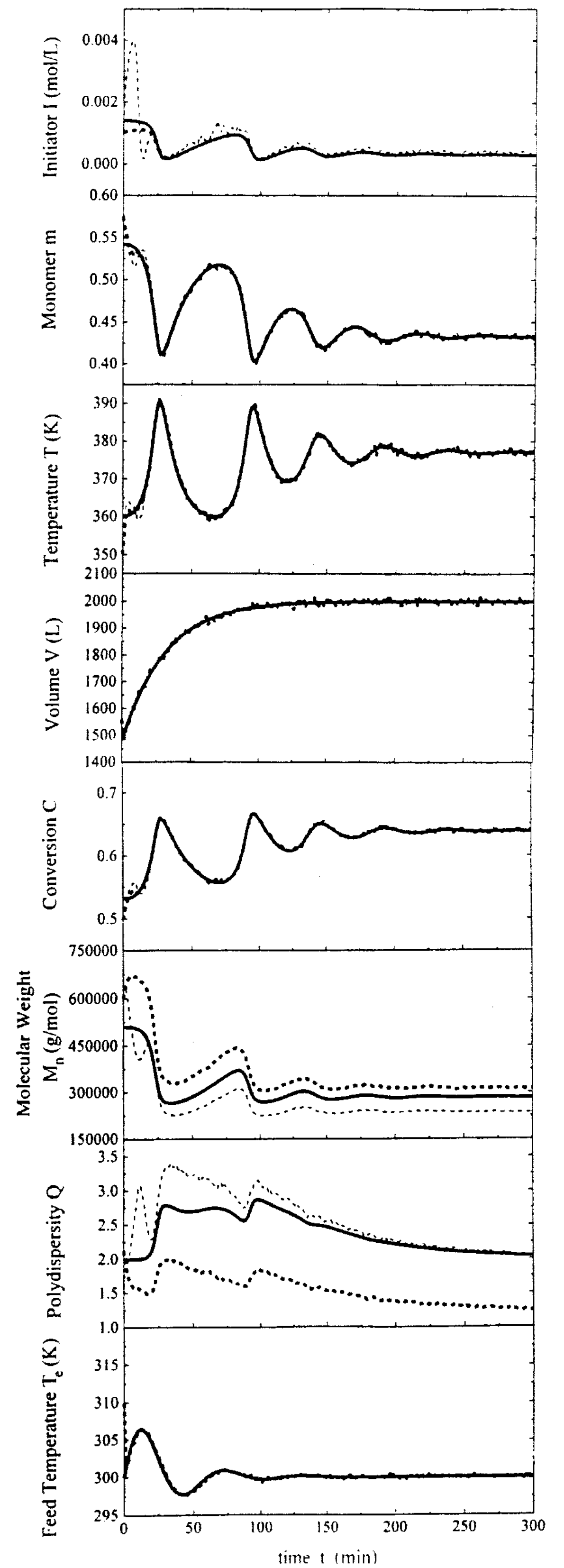

Figure 5b. Evolutions of the reactor (——), and *PI* estimators run with model parameter errors and noisy measurements of Figure 5a for Cases 1 ($\kappa = 3$:---) and 2 ($\kappa = 4$:---).

Concluding remarks

From the preceding series of tests, the best performance-robustness trade-off was obtained with the PI-estimator with the observability index set $\kappa_2 = \{2, 1, 1\}$. With model parameter errors and noisy measurements, the conversion converges with zero mean and a small standard deviation offset, the molecular weight converges with some offset and a very small standard deviation, and the polydispersity converges with a very small offset and a small standard deviation. From a practical viewpoint, the convergence offsets of the average molecular weight (M_n) and its polydispersity (Q) are acceptable, given that they are smaller than the standard deviation of on-line measurement devices. Should the convergence offsets of M_n and Q be unacceptably large, two things can be done to improve them. One possibility is to fit some kinetic parameters to match the predictions of M_n and Q; the other possibility is to extend the proposed estimation scheme to incorporate on-line chromatographic, discrete-delayed measurements of M_n and Q, as has been done in the nonlinear EKF design of Schuler and Sushen (1985).

Conclusions

A dynamic state-estimation technique for MIMO nonlinear plants has been presented. In contrast to the EKF and HG nonlinear observation techniques, the proposed design applies to plants that are either observable or detectable, thus considerably broadening its applicability. The estimator design stems from a geometric-type definition of nonlinear estimability that includes a flatness feature that enables a coordinate change with measurement injection so that the resulting output error dynamics are quasi-linear, noninteractive, and pole-assignable. In this way, the tuning of gains and the interpretation of the functioning of the estimator can be done with conventional filtering and control techniques for linear single input, single output (SISO) systems, identical to the ones employed in industrial practice. The design includes an estimability property that can be assessed *a priori* (before construction and tuning) and whose structure is a design degree of freedom. The design features a robust convergence criterion coupled with a systematic construction-tuning procedure, and it has a framework where the nature of the compromise between the performance and the robustness of the estimator is identified. In principle, the methodological approach of the present design can be extended to study the choice of the on-line numerical integration scheme, and to study the case when the measurements are taken at discrete time intervals.

The present design offers these advantages with respect to previous approaches: (1) it is not restricted to observable plants, as the EKF, HG, and GO designs are; (2) its applicability is far less restrictive than the one of the GO design; (3) it is free of the burdensome on-line solution of a nonlinear Riccati-type matrix equation, and of the trial-and-error approach to the tuning of gains, which both characterize the EKF technique; and (4) that it provides a means to systematize the *ad hoc* estimators tailored for specific plants.

The proposed estimation design was applied to a class of free-radical homopolymerization reactors. The solvability of the estimation problem was assessed *a priori* in terms of conditions bearing physical meaning, whose consequence was that the construction-tuning stage turned into a straightforward task. The application example showed that the estimator design can benefit, in an essential way, from the assistance of polymer reaction engineering tools in particular, and of chemical process engineering tools in general.

As pointed out in the introduction, the observability or detectability property of a plant depends on the presence and kind of feedback controller. If some of the inputs of the plant are generated by a (possibly conventional) feedback controller that is not driven by an estimator, the proposed estimation design should just be applied to the corresponding closed-loop plant, replacing the exo-observer for the controlled inputs with the feedback equation, and retaining the exo-observer for the exogenous noncontrol inputs. If the plant is subjected to an estimator-based controller, a suitable RE-stable state-feedback controller should be designed first, the proposed estimation design should be applied to the closed-loop plant, and the RE-stability of the plant-estimator interconnection should be guaranteed. In particular, the combination of the proposed estimator with a nonlinear geometric controller should lead to the robust version of the nominally convergent estimator-based nonlinear geometric controller presented in Alvarez (1996).

Acknowledgments

Part of this work was accomplished during the sabbatical stay of J. Alvarez at Comerical Mexicana de Pinturas, Centro de Investigación en Polímeros (CIP). T. López received support from the Mexican National Council for Research and Technology (CONACYT) and the CIP Award for Graduate Studies.

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Appendix A: Matrices, Vectors, and Nonlinear Maps

Vectors and matrices

$bd\ M :=$ a block-diagonal matrix M

$$\Gamma_{u/o} = bd\left[\Gamma_1^{u/o}, \ldots, \Gamma_{p/m}^{u/o}\right], \qquad \Pi_{u/o} = bd\left[\pi_1^{u/o}, \ldots, \pi_{p/m}^{u/o}\right],$$

$$\Delta_{u/o} = bd\left[\delta_1^{u/o}, \ldots, \delta_{p/m}^{u/o}\right]$$

$$\Gamma^{u/o}_{i(\nu_i \times \nu_i)/(\kappa_i \times \kappa_i)} = \begin{bmatrix} 010\cdots 0 \\ \vdots \qquad \vdots \\ 0\ \cdots 0\ 1 \\ 0\ \cdots\ 0 \end{bmatrix}, \qquad \pi^{u/o}_{i(\nu_i \times 1)/(\kappa_i \times 1)} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix},$$

$$\delta^{u/o}_{i(1 \times \nu_i)/(1 \times \kappa_i)} = [1, 0, \ldots, 0]$$

$$A_{u/o} = \Gamma_{u/o} - K_{u/o}\Delta_{u/o}, \qquad A_o^e = \Gamma_o^e - K_o^e\Delta_o^e,$$

$$\Gamma_o^e = bd[\Gamma_1^e, \ldots, \Gamma_m^e], \qquad \Delta_o^e = bd[\delta_1^e, \ldots, \delta_m^e]$$

$$\Pi_o^e = bd[\pi_1^e, \ldots, \pi_m^e], \qquad \Gamma_i^e = \Gamma^o_{i(\kappa_i+1)\times(\kappa_i+1)},$$

$$\delta_i^e = (\delta_i^o, 0), \qquad \pi_i^e = (\pi_i^{o\prime}, 0)'$$

$$K_o^e = bd\Big[\big(s_o k_{11}^o, \ldots, s_o^{\kappa_1} k_{\kappa_1 1}^o, s_o^{\kappa_1+1} k_1^I\big)', \ldots,$$
$$\big(s_o k_{1m}^o, \ldots, s_o^{\kappa_m} k_{\kappa_m m}^o, s_o^{\kappa_m+1} k_m^I\big)'\Big]$$

$$T[e_I', e_q']' = [e_1^I, \ldots, e_{\kappa_1}^I, e_1^q; \ldots; e_{\kappa_{m-1}}^I, \ldots, e_\kappa^I, e_m^q]';$$

$$e_I = [e_1^I, \ldots, e_{\kappa_1}^I; \ldots, e_{\kappa_{m-1}}^I, \ldots, e_\kappa^I]', \quad e_q = [e_1^q, \ldots, e_m^q]'.$$

Nonlinear maps

$$\theta(z, \upsilon, r) = \{\varphi(x, x_u, \dot{x}_u, r)\}_{[x=\phi^{-1}(z,r),\ x_u = z_u,\ \dot{x}_u = \Gamma_u z_u + \Pi_u \upsilon]},$$

$$z = (z_u', z_I', z_{II}')'$$

$$w(z, \upsilon, r)$$

$$= [(\partial\phi_{II}/\partial x) f + (\partial\phi_{II}/\partial u\dot{x}_u)]_{[x=\phi^{-1}(z,r),\ x_u = z_u,\ \dot{x}_u = \Gamma_u z_u + \Pi_u \upsilon]}$$

$$\omega(e_{II}, t) = \{w[(z_u', z_I', z_{II}' + e_{II})', \upsilon, r] - w(z, \upsilon, r)\}_{[z(t),\ \upsilon(t)]}$$

$$q_I(e_u, e_I, e_{II}, \upsilon, e_r, t) = [\theta(z+e, \upsilon, r+e_r) - \theta(z, \upsilon, r)]_{[z(t),\ \upsilon(t)]}$$

$$q_{II}(e, \upsilon, e_r, t) = \{w(z+e, \upsilon, r+e_r) - w[(z_u', z_I', z_{II}' + e_{II})', \upsilon, r]\}_{[z(t),\ \upsilon(t)]}$$

$$q_s(e_{II}, e_r, t) = q_I(0, e_{II}, 0, e_r, t),$$

$$q_f(e_I, e_u, t) = q_I(e_I, e_{II}, e_u, e_r, t) - q_I(0, e_{II}, 0, e_r, t).$$

Appendix B: Proofs of Theorem and Corollary 2

Proof of Theorem 2. First subtract the augmented plant (Eq. 7) from its PI-estimator (Eq. 26), then apply the flattening coordinate-change (Eq. 10), incorporate the dynamics (Eq. 22) for the new state x_q, substitute Eq. 22, and, finally, obtain the following error dynamics ($e_q = \chi_q - x_q . q_f$ and q_s are defined in Appendix A):

$$\dot{e}_u = A_u e_u - \Pi_u \upsilon(t), \qquad \dot{e}_q = -K_I \Delta_o e_I,$$

$$\dot{e}_I = A_o e_I + \Pi_o \{q_f(e_I, e_u, t) + q_s(e_{II}, e_r, t) + e_q\}$$

$$\dot{e}_{II} = \omega(e_{II}, t) + q_{II}[e, e_u, \upsilon(t), e_r, t],$$

$$\mu = \Delta_u e_u, \qquad \upsilon = \Delta_o e_u$$

or equivalently, Eq. 28. Compare this equation set with the one (Eq. 12) of the P-estimator, recall that $\|\Pi_o^e\| = \|\Pi_o\| = 1$, and conclude that the preceding error dynamics are RE-stable if the inequality condition (Eq. 20) of Theorem 1 is met when the pair (a_o, λ_o) is replaced with (a_o^e, λ_o^e), or equivalently, when the conditions of Theorem 2 are met. QED

Proof of Corollary 2. From the comparison argument utilized in the final part of the proof of Theorem 2, it follows that the PI-estimator RE-converges with the equality sets of Corollary 1 when the set $\{a_o, \lambda_o, A_a, L_a\}$ is replaced with $\{a_o^e, \lambda_o^e, A_a^e, L_a^e\}$. QED

Appendix C: Proof of Proposition 1

Proof of Proposition 1. From Definition 1 and the reactor model (Eq. 32), it follows that, for any observability index set $\mathbb{k} = \{\kappa_1, \kappa_2, \kappa_3\}$, the map ϕ_I is L-continuous and independent of μ_0 and μ_2, implying that these states are unobservable. Hence, the integer κ can be either 3 or 4, with the four pairs $(\mathbb{k}, \phi_I)$ listed in statements (ii) and (iii) of Proposition 1, and the following unobservable surfaces and L-continuous maps φ [dim $\Xi_1(t) = 3$, dim $\Xi_i(t) = 2$, $i = 2, 3, 4$]:

$$\Xi_1(t) = \{x \in X \mid (m, T, V) = (y_1, y_2, y_3)(t)\},$$

$$\Xi_2(t)\{x \in X \mid (m, f_m, T, V) = (y_1, \dot{y}_1, y_2, y_3)'(t)\}$$

$$\Xi_3(t) = \{x \in X \mid (m, T, f_T, V) = (y_1, y_2, \dot{y}_2, y_3)(t)\},$$

$$\Xi_4(t) = \{x \in X \mid (m, T, V, f_V) = (y_1, y_2, y_3, \dot{y}_3)(t)\}$$

$$\varphi = (f_m, f_T, f_\upsilon)'(x, u) \quad \text{for} \quad \mathbb{k}_1,$$

$$(L_f f_m, f_T, f_V)' \quad \text{for} \quad \mathbb{k}_2,$$

$$(f_m, L_f f_T, f_V)' \quad \text{for} \quad \mathbb{k}_3, \quad (f_m, f_T, L_f f_V)' \quad \text{for} \quad \mathbb{k}_4.$$

For $\mathbb{k}_1$ the map ϕ_{II} of statement (ii) yields the trivially Rx-invertible identity map $\phi = x$, and the unobservable dynamics of statement (ii), whose motions are RE-stable because they do not contain the monomer dynamics. Hence, the reactor motions are RE-detectable with $\mathbb{k}_1$.

From the physical property $\partial r_p/\partial I > 0$ and the reactor model, it follows that

$$\partial f_m/\partial I = -(1-\epsilon_m)(\partial r_p/\partial I) < 0,$$

$$\partial f_T/\partial I = \beta(m)(\partial r_p/\partial I) > 0, \qquad \partial f_\upsilon/\partial I = -\epsilon V(\partial r_p/\partial I) < 0,$$

implying that f_m, f_T, and f_V are RI-invertible maps, or equivalently, that the three maps ϕ of statement (iii) are Rx-invertible. Thus, at each time, the observable state I is determined by any of the three equations $f_m = \dot{y}_1$, $f_T = \dot{y}_2$, or $f_V = \dot{y}_3$. This means that the observability index sets $\mathbb{k}_2$, $\mathbb{k}_3$, and $\mathbb{k}_4$ determine the same unobservable surface Ξ (i.e., $\Xi_2 = \Xi_3 = \Xi_4 := \Xi \subset \Xi_1$), with the unobservable dynamics of statement (iii). The RE-stability of their unobservable motions follows from the fact that the unobservable surface Ξ is contained in the one (Ξ_1) of the case with $\mathbb{k}_1$. Thus, the reactor motions are RE-detectable with $\mathbb{k}_2$, $\mathbb{k}_3$, and $\mathbb{k}_4$. QED

Manuscript received May 19, 1998, and revision received Sept. 20, 1998.