ON-LINE MONITORING OF A COPOLYMER REACTOR: A CASCADE ESTIMATION DESIGN

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Abstract: In this work the problem of on-line monitoring of product quality and production rate in a copolymer reactor is addressed, using an estimation scheme with secondary measurements of density, refractive index, temperature, and volume. Three different estimator structures are studied: (a) the nominal detectability structure that underlines the extended Kalman filter and Luenberguer observers, (b) a passive estimation structure with estimation degrees equal to one, and (c) a hybrid structure that combines the detectability and passive structures in low and high gain, respectively. The nominal detector maximizes the reconstruction rate, the passive estimator maximizes the robustness, and the cascade (hybrid) design achieves a suitable compromise between them. The approach is illustrated with a copolymer reactor case and simulations.

Keywords: Chemical industry, Monitoring, Extended Kalman filter, Geometric approach, Observability, Detectors, State estimation.

1. INTRODUCTION

Copolymerization is an important industrial process where commodity and engineering plastics are manufactured. In a continuous reactor operation, the knowledge of the instantaneous copolymer properties (such as copolymer composition, conversion, mass fraction, molecular weight, etc.) is important for on-line monitoring, control, and fault detection purposes. These properties have direct implications in the safety, product quality and production rate performance indices, but they are not available on-line. Thus, the estimation objective is the inference of variables related to product quality and production rate using a model-based estimation technique with secondary on-line measurements (Mutha et al., 1997; Dimitratos et al., 1991; Ellis et al, 1994; Van Dooting et al., 1992).

In polymer reactor engineering, the Extended Kalman Filter (EKF) is the most widely used state estimation technique, and the Luenberguer observer (LO) has been increasingly considered in the last decade. In both techniques, their structure is fixed and determined by the nominal observability property. If this property is ill-conditioned, any appropriately constructed and tuned detector should diverge or malfunction. To tackle this problem, the idea of considering the estimator structure as a degree of freedom to improve its functioning was proposed in the geometric estimation design (Alvarez and Lopez, 1999; Alvarez, 2000). In Hernandez and Alvarez (2003), the corresponding definition of nonlinear estimability (a robust form of detectability) was put in formal perspective with the existing indistinguishability-based definitions of nonlinear detectability (Hermann and Krener, 1977; Sontag, 1990). In Alvarez and Lopez (2003), the effect of the estimator structure on its functioning was studied for a representative case study of a copolymer reactor, showing that: (i) the structure decision problem is not trivial in the sense that there are 56 possible estimator structures for the case study; (ii) the best functioning is attained neither with the nominal detectability structure associated with the standard EKF and LO nor with a passive estimation structure (i.e. with estimation degrees equal to one), but with an intermediate structure; and (iii) how the estimation structure determines the estimator reconstruction rate and the error propagation mechanism.

Having as a point of departure the aforementioned results on the copolymer reactor case (Lopez and Alvarez, 2003), in this work the problem of on-line inferring the safety, quality and production rate is addressed. Using the geometric estimation approach with secondary measurements of density, refractive index, temperature, and volume. Considering that the nominal detector maximizes the innovated dynamics dimension and therefore the reconstruction rate, and that the passive estimator maximizes the robustness to modeling errors. Here the idea is to use a hybrid structure that superimposes a fast passive estimator with the slow nominal detector, obtaining a cascade estimator that yields a better compromise between reconstruction rate and robustness. The three estimator designs (nominal detector, passive estimator and cascade design) are illustrated with a copolymer reactor case and simulations.

2. THE COPOLYMER REACTOR PROBLEM

2.1 The reactor model

Let us consider a continuous reactor where a solution copolymerization takes place (see Fig. 1). The reactions are strongly exothermic, and heat is removed by means of a cooling jacket. There is significant gel-effect (i.e., reaction autoacceleration by diffusional limitations in the mobility of the copolymer chains), meaning a copolymer conversion accompanied by a considerable viscosity increase and a decrease in the heat exchange capability. From standard kinetics, reaction engineering, and viscous heat exchange modeling considerations, the reactor model is given as follows (functions and parameters defined in Padilla and Alvarez, 1996):

$$\dot{m}_1 = -r_1 + (q_1 m_{1e} - q_e m_1)/V := f_1(m_1,m_2,p_1,p_2,i,T,V)$$

$$\dot{m}_2 = -r_2 + (q_2 m_{2e} - q_e m_2)/V := f_2(m_1,m_2,p_1,p_2,i,T,V)$$

$$\dot{p}_1 = -r_1(1-\varepsilon_1) + (q_1 p_{1e} - q_e p_1)/V := f_3(m_1,m_2,p_1,p_2,i,T,V)$$

$$\dot{p}_2 = -r_2(1-\varepsilon_2) + (q_2 p_{2e} - q_e p_1)/V := f_4(m_1,m_2,p_1,p_2,i,T,V)$$

$$\dot{i} = -r_I + (w_I - q_e i)/V := f_5(i,T,V)$$

$$\dot{T} = r_T - \gamma(T-T_c) + q_{he} - q_h := f_6(m_1,m_2,p_1,p_2,i,T,V)$$

$$\dot{V} = q_e - q := f_7(m_1,m_2,p_1,p_2,i,T,V)$$

$$\dot{\mu}_0 = r_{\mu 0} + [(q_1+q_2)\mu_{0e} - q_e\mu_0]/V := f_8(m_1,m_2,p_1,p_2,i,T,V,\mu_0)$$

$$\dot{\mu}_2 = r_{\mu 2} + [(q_1+q_2)\mu_{2e} - q_e\mu_2]/V := f_9(m_1,m_2,p_1,p_2,i,T,V,\mu_2)$$

where

$$q_e = q_1\phi_1 + q_2\phi_2 + q_s\phi_s + (r_1\phi_4 + r_2\phi_5)V$$

$$q_h = (q_1\rho_1 + q_2\rho_2 + q_s\rho_s)T/(\rho V)$$

$$q_{he} = (q_1\rho_1 C_{p1} T_{1e} + q_2\rho_2 C_{p2} T_{2e} + q_s\rho_s C_{ps} T_{se})/(\rho V C_p)$$

The reactor states (x) are: the dimensionless concentrations (referred to pure materials) of the i-th monomer (m_i), of the i-th converted monomer (p_i), and of the initiator (i); the temperature (T), the volume (V), and the zeroth (μ_0) and second (μ_2) moments of the chain length distribution (CLD). The exogenous inputs (u) are: the feed concentration of i-th monomer (m_{ie}), and of the i-th converted monomer (p_{ie}); the feed temperatures of the i-th monomer (T_{ie}), and of the solvent (T_{se}); the jacket temperature (T_c), the feed flowrate of the i-th monomer (q_i), and of the solvent (q_s); the mass feedrate of initiator (w_{Ie}); and the exit flowrate (q). The total feed flowrate (q_e) is corrected by the contraction of volume due to the polymerization, where (ϕ_1, ϕ_2, ϕ_3, ϕ_4, ϕ_5) is equal to (1, 1, 1, 0, 0) if no volume contraction is considered. While the dimensionless solvent concentration (s) is given by

$$s = 1 - (m_1 + m_2 + p_1 + p_2)$$

The following set of scalar fields are smooth and strictly positive: the rates of initiator decomposition (r_I), polymerization of monomers 1 (r_1) and 2 (r_2), and change of the zeroth ($r_{\mu 0}$) and second ($r_{\mu 2}$) CLD moments, the ratios of heat generation (r_T) and exchange (γ) to heat capacity, the input (q_{he}) and the output (q_h) enthalpy flows. The measured outputs (y) are the density (ρ), the refractive index (η), the temperature (T), and the volume (V):

$$y_1 = \rho, \qquad y_2 = \eta, \qquad y_3 = T, \qquad y_4 = V$$

where ρ is calculated by volume additivity and η according the Lorimer theory (1972):

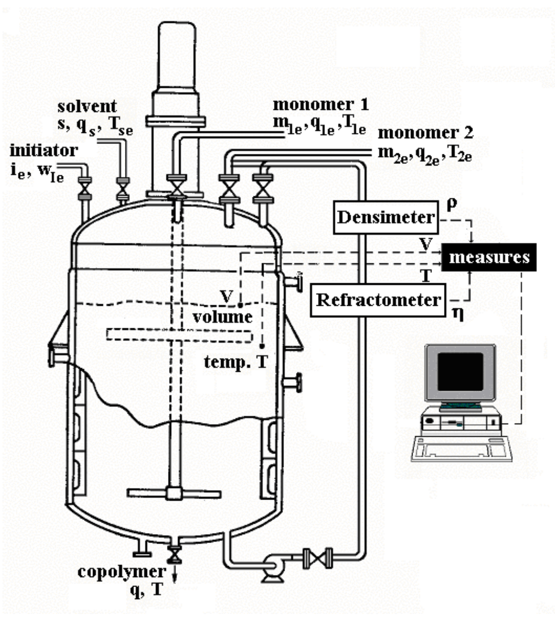

Fig. 1. The copolymerization reactor.

$\rho = m_1\rho_1^o + m_2\rho_2^o + p_1\rho_1^p + p_2\rho_2^p + s\rho_s^o := h_1(m_1,m_2,p_1,p_2)$

$\eta = \eta_o + C_s\nu + a_2C_s^2 := h_2(m_1,m_2,p_1,p_2)$

The outputs (z) to be inferred are: the instantaneous composition (z_c) of monomer 1, the conversion (z_p) of copolymer, the weight-average molecular weight (z_M) of the CLD, and the production rate (z_R) of copolymer:

$z_c = r_1M_1^o / (r_1M_1^o + r_2M_2^o) := g_1(m_1, m_2, p_1, p_2, i, T)$

$z_p = (p_1P_1^o + p_2P_2^o) / (m_1M_1^o + m_2M_2^o + p_1P_1^o + p_2P_2^o)$
$:= g_2(m_1, m_2, p_1, p_2)$

$z_M = \mu_2 / (p_1P_1^o + p_2P_2^o) := g_3(p_1, p_2, \mu_2)$

$z_R = (r_1\rho_1^o + r_2\rho_2^o)V := g_4(m_1, m_2, p_1, p_2, i, T)$

which are key variables to monitor the product quality and the production rate.

In compact notation, the reactor model can be as follows:

$$\dot{x} = f(x, u, p), \qquad y = h(x, p), \qquad z = \eta(x, p) \qquad (1)$$

where p is the vector of model parameters, and

$x = [m_1, m_2, p_1, p_2, i, T, V, \mu_0, \mu_2]^T$

$y = [y_\rho, y_\eta, y_T, y_T]^T$

$u = [m_{1e},m_{2e},p_{1e},p_{2e},T_{1e},T_{2e},T_{se},T_c,q_1,q_2,q_s,w_{Ie},q]^T$

$z = [z_c, z_p, z_M, z_R]^T$

2.2 Reactor dynamics

As a case study, the copolymerization of methyl methacrylate (MMA) and vinyl acetate (VAC) is considered, with ethyl acetate (AE) as solvent and azo-bis-isobutyronitrile (AIBN) as initiator. In steady-state operation, the copolymer reactor may exhibit multiplicity of critical points (Hamer *et al.*, 1981). The nominal input

$u = [1.0, 1.0, 0.0, 0.0, 315\text{ K}, 315\text{ K}, 315\text{ K}, 328\text{ K}, 1.11\text{x}10^{-3}\text{ m}^3/\text{min}, 6.23\text{x}10^{-3}\text{ m}^3/\text{min}, 1.99\text{x}10^{-3}\text{ m}^3/\text{min}, 6.66\text{x}10^{-5}\text{ Kmol/min}, 8.53\text{x}10^{-3}\text{ m}^3/\text{min}]^T$

was chosen such that the reactor had three steady-states: two of them (ignition and extinction-type) are stable, and one is unstable. To test the functioning of

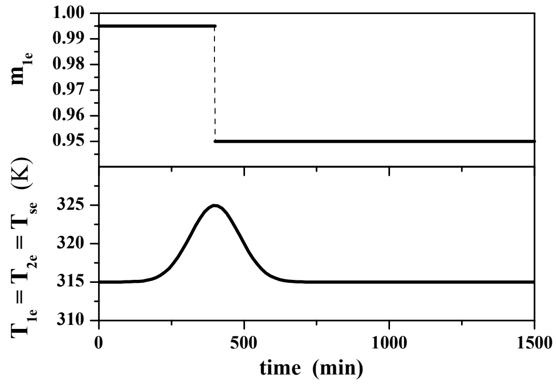

Fig. 2. Time-varying exogenous inputs.

the proposed estimation designs, the following reaction motion was considered. Initially, the reactor is at its unstable steady-state, and the four exogenous inputs $u(t) = [m_{1e}(t), T_{1e}(t), T_{2e}(t), T_{se}(t)]^T$ are varied as shown in Fig. 2. As a result, the reactor is driven to its ignition-type steady-state after undergoing a transient with ample and abrupt changes in its state, as it can be seen in the continuous thick curves of Fig. 4. This drastic motion must be regarded as the extreme case of a practical situation, in order to subject the proposed estimation scheme to a severe test.

2.3 The on-line monitoring problem

Our main objective is the on-line inference of the variables (z) related to product quality (instantaneous composition, conversion and molecular weight) and production rate, using a robust estimation design with on-line secondary measurements (y) of density, refractive index, temperature, and volume.

As mentioned before, this reactor admits 56 estimator structures (Lopez, 2000; Alvarez and Lopez, 2003), including the nominal detectability structure associated to the standard EKF and LO designs. However the best functioning is attained nor with the nominal detectability structure either with a passive structure, but with an intermediate one. Here, a constructive-like framework (Sepulchre *et al.*, 1997) is recalled to design a cascade estimator to improve its behavior: a low gain detectability structure is cascaded to a high gain passive structure in order to obtain a better compromise between reconstruction rate and robustness to modeling errors.

3. NONLINEAR ESTIMATION

In this section, the notions of nominal and robust nonlinear detectability are defined according Alvarez and Lopez (1999) and Hernandez and Alvarez (2003). The construction of the geometric high-gain observer follows from a straightforward consequence of the detectability property. The estimator construction, the convergence criterion, and the tuning technique can be found in Alvarez and Lopez (1999) and Alvarez (2000). Then, the nominal and passive structures of the copolymer reactor case are recalled (Lopez, 2000; Lopez and Alvarez, 2003). Then, the cascade structure is introduced and justified. Finally, three estimator designs are presented and compared: the nominal detector, the passive estimator and the cascade design.

3.1 Detectable and passive structures

From Lopez (2000) and Lopez and Alvarez (2003), we know that the copolymer reactor [Eq. (1)] motion is nominally detectable (i.e. the observability matrix has maximum rank) with the structure:

$$S_D = (\underline{k}, x_o, x_\mu) \tag{2}$$

where $\underline{k}$ is the observability index vector, and x_o (or x_μ) is the observable (or unobservable) state:

$$\underline{k} = (k_1, k_2, k_3, k_4) = (2, 2, 2, 1), \quad k = \sum k_i = 7 \tag{3a}$$

$$x_o = [x_1, \ldots, x_7]^T = [m_1, m_2, p_1, p_2, i, T, V]^T \tag{3b}$$

$$x_\mu = [x_8, x_9]^T = [\mu_0, \mu_2]^T \tag{3c}$$

This detectability property with partial observability follows from the fulfillment of two conditions: (i) the observability matrix O has rank 7 over time, and (ii) the unobservable motion x_μ (t) is stable. This is,

$$\text{Rank } O(x, u, p, \underline{k}) = 7 \quad \forall\, t \tag{4a}$$

$$O(x, u, p, \underline{k}) = \partial\phi/\partial x_o, \qquad \dim O = k = 7 \tag{4b}$$

$$\phi(x, u, p, \underline{k}) = [h_1, (\partial h_1/\partial x)\, f, h_2, (\partial h_2/\partial x)\, f, x_6, f_6, x_7]^T$$

and the unobservable dynamics

$$\dot{x}^*_\mu = [f_8, f_9]^T[\phi^{-1}(u, p, \underline{k}), x^*_\mu, u, p] := f_\mu(x_o, x^*_\mu, u, p) \tag{5a}$$

have a (unique) stable solution

$$x^*_\mu(t) = \theta_\mu(t, t_0, x^*_{\mu 0}, u, p, \underline{k}) \tag{5b}$$

The nominal detectability structure S_D [Eq. (2)] is the one that, over the set of 56 admissible structures, maximizes the dimension of the innovated (i.e., with measurement injection) dynamics, or equivalently, the reconstruction rate, regardless of robustness considerations. If the observability matrix [Eq. (4b)] is ill-conditioned, any nominal detectability-based observer should malfunction or diverge.

In the spirit of the passivation backstepping procedure (Sepulchre *et al.*, 1997; Kristic *et al.*, 1995), let us recall the passive structure (Lopez and Alvarez, 2003)

$$S_P = (\underline{\kappa}, x_I, x_{II}) \tag{6}$$

that maximizes the robustness at the cost of the reconstruction rate. $\underline{\kappa}$ is the estimation degree vector, and x_I (or x_{II}) is the innovated (or non-innovated) state:

$$\underline{\kappa} = (\kappa_1, \kappa_2, \kappa_3, \kappa_4) = (1, 1, 1, 1), \quad \kappa = \sum \kappa_i = 4 \tag{7a}$$

$$x_I = [x_1, x_2, x_6, x_7]^T = [m_1, m_2, T, V]^T \tag{7b}$$

$$x_{II} = [x_3, x_4, x_5, x_8, x_9]^T = [p_1, p_2, i, \mu_0, \mu_2]^T \tag{7c}$$

This estimability property (with minimum innovation) follows from the fulfillment of two conditions: (i) the innovation matrix O has rank 4 over time, and (ii) the non-innovated motion $x_{II}(t)$ is stable. This is,

$$\text{Rank } O(x, u, p, \underline{\kappa}) = 4 \quad \forall\, t \tag{8a}$$

$$O(x, u, p, \underline{\kappa}) = \partial\phi/\partial x_I, \qquad \dim O = \kappa = 4 \tag{8b}$$

$$\phi(x, u, p, \underline{\kappa}) = [h_1, h_2, x_6, x_7]^T$$

and the non-innovated dynamics

$$\dot{x}^*_{II} = [f_3, f_4, f_5, f_8, f_9]^T[\phi^{-1}(u, p, \underline{\kappa}), x^*_{II}, u, p]$$
$$:= f_{II}(x_I, x^*_{II}, u, p) \tag{9a}$$

have a (unique) stable solution

$$x^*_{II}(t) = \theta_{II}(t, t_0, x^*_{II0}, u, p, \underline{\kappa}) \tag{9b}$$

Figure 3 shows the condition number of the observability (or innovation) matrix [Eqs. (4b) or (8b)] associated to the nominal detectability (or passive) structure S_D (or S_P), showing that the observability matrix is significantly more ill-conditioned (by 5 order of magnitude) than the passive innovation matrix.

3.3 Cascade structure

In the adjustable structure estimation study presented in Lopez and Alvarez (2003), it was established that the best estimator behavior was attained with an intermediate degree (k = 5) structure, and not with the detectability (k = 7) or passive (κ = 4) structure. In the understanding that the detectability structure is the one that underlies the well known nonlinear EKF and LO. Motivated by the structure-oriented nonlinear constructive control approach (Sepulchre *et al.*, 1997; Kristic *et al.*, 1995), in the present work a different way to obtain a better estimator behavior is considered: the cascade combination of a low gain detectability structure with a high gain passive structure. According to the following rationale: (i) first, a high-gain passive estimator (i.e, with fast dynamics) is designed in order to quickly and robustly match the input-output reactor behavior, regarding this estimator as a redesigned model, and then (ii) a low-gain nominal detector is designed for this new model, in order to reconstruct the maximum number of states. This idea has been applied successfully in a catalytic reactor with experimental data (Lopez *et al.*, 2002). However in this catalytic reactor the structure estimation choice was not a complex task because there are only two candidate structures. While in our copolymer reactor case there are 56 admissible estimation structures.

To define the cascade structure, let us consider the following state partition:

$$x = [x_I, x_P, x_\mu]^T \tag{10a}$$

$$x_I = [x_1, x_2, x_6, x_7]^T = [m_1, m_2, T, V]^T \tag{10b}$$

$$x_P = [x_3, x_4, x_5]^T = [p_1, p_2, i]^T \tag{10c}$$

$$x_\mu = [x_8, x_9]^T = [\mu_0, \mu_2]^T \tag{10d}$$

where x_P is made by the observable states [Eq. (3b)] transferred from the observable state (x_o) to the non-innovated one (x_{II}).

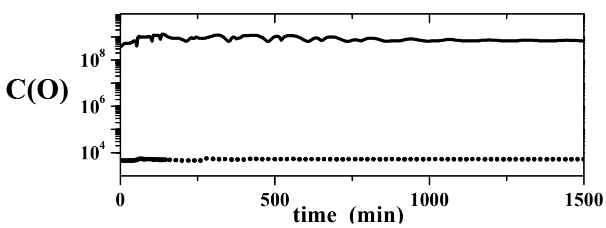

Fig. 3. Condition number C(O) of the observability (——) or innovation (.....) matrices [Eqs. (4b) or (8b)] associated to the detectability (S_D) and passive (S_P) structures.

3.4 Estimators

Nominal detector. The PI (proportional - integral) estimator construction follows from a straightforward application of Theorem 2 given in Alvarez and Lopez (1999), obtaining the following nominal detector:

$$\dot{\hat{x}}_o = f_o(\hat{x}, u, \hat{p}) + G(\hat{x}, u, \hat{p}, \underline{k}, s)\,[y - h(\hat{x}, \hat{p})]$$
$$+ H(\hat{x}, u, \hat{p}, \underline{k}) \int K_I(\underline{k}, s)[y - h(\hat{x}, \hat{p})]dt \qquad (11a)$$
$$\dot{\hat{x}}_\mu = f_\mu(\hat{x}, u, \hat{p}) \qquad (11b)$$
$$\hat{y} = h(\hat{x}, \hat{p}), \quad \hat{z} = g(\hat{x}, \hat{p}), \quad \hat{x} = [\hat{x}_o, \hat{x}_\mu]^T \qquad (11c)$$

Here the nonlinear gains are given by

$[G, H]\,(\hat{x}, u, \hat{p}, \underline{k}, s) = O^{-1}(\hat{x}, u, \hat{p}, \underline{k})\,[K_p(\underline{k}, s), \Pi(k)]$

O^{-1} is the inverse of the observability matrix, and $\{\Pi, K_P, K_I\}$ are given by (bd := block diagonal)

$\Pi(k) = bd[\pi_1, \pi_2, \pi_3, \pi_4]$, $\dim \Pi = k \times 4$

$K_P(k, s) = bd[k_{p1}, k_{p2}, k_{p3}, k_{p4}]$, $\dim K_P = k \times 4$

$K_I(k, s) = diag[(s\omega_1)^{k_1+1}, (s\omega_2)^{k_2+1}, (s\omega_3)^{k_3+1}, (s\omega_4)^{k_4+1}]$

$\pi_i = [1]$, $k_{pi} = [s\omega_i]$ if $k_i = 1$

$\pi_i = [0, 1]^T$, $k_{pi} = [(2\zeta+1)s\omega_i, (2\zeta+1)(s\omega_i)^2]^T$ if $k_i = 2$

where (ω_i, ζ, s) are the output reference frequencies (one for each measurement), the reference damping factor, and the celerity estimator parameter, which are considered as tuning parameters.

Passive estimator. In this case the design is equivalent to previous estimator [Eqs. (11)] but replacing the observability index vector $\underline{k}$ [Eq. (3a)] by $\underline{\kappa}$ [Eq. (7a)], the observability matrix O [Eq. (4b)] by the innovation one [Eq. (8b)], the state partition [Eqs. (3b) and (3c)] by [Eqs. (7b) and (7c)], and the unobservable dynamics [Eq. (5a)] by the non-innovated dynamics [Eq. (9a)].

Cascade design. The application of the construction guidelines given in the previous subsection yields the cascade estimator:

$$\dot{\hat{x}}_I = f_I(\hat{x}, u, \hat{p}) + [G(\hat{x}, u, \hat{p}, \underline{\kappa}, s_f) +$$
$$G(\hat{x}, u, \hat{p}, \underline{k}, s_s)]\,[y - h(\hat{x}, \hat{p})] + [H(\hat{x}, u, \hat{p}, \underline{\kappa})K_I(\underline{\kappa}, s_f)$$
$$+ H(\hat{x}, u, \hat{p}, \underline{k})K_I(\underline{k}, s_s)] \int [y - h(\hat{x}, \hat{p})]dt \qquad (12a)$$
$$\dot{\hat{x}}_P = f_P(\hat{x}, u, \hat{p}) + G(\hat{x}, u, \hat{p}, \underline{k}, s_s)\,[y - h(\hat{x}, \hat{p})]$$
$$+ H(\hat{x}, u, \hat{p}, \underline{k})\, K_I(\underline{k}, s_s) \int [y - h(\hat{x}, \hat{p})]dt \qquad (12b)$$
$$\dot{\hat{x}}_\mu = f_\mu(\hat{x}, u, \hat{p}) \qquad (12c)$$
$$\hat{y} = h(\hat{x}, \hat{p}), \quad \hat{z} = g(\hat{x}, \hat{p}), \quad \hat{x} = [\hat{x}_I, \hat{x}_p, \hat{x}_\mu]^T \qquad (12d)$$

where s_s (or s_f) is the slow (or fast) celerity parameter that sets the convergence rate of the associated passive estimator (or detector). In this way, the convergence rate of x_I (or x_P) is affected by (s_s, s_f) (or s_s), and the convergence rate of the non-innovated state x_μ is independent of (s_s, s_f).

The convergence conditions for the detector and passive estimators [Eqs. (11)] are given in Alvarez and Lopez (1999). The technical derivation of the convergence criterion of the proposed cascade design [Eqs. (12)] goes beyond the scope of the present work. Here, it suffices to say that the application of the singular perturbation arguments employed in standard cascade control design yields that the proposed cascade estimator is convergent if: (i) first, with the slow parameter defined ($s_s = 0$), the parameter s_f is tuned sufficiently fast (typically 3 to 15 times the reactor natural dynamics) so that the passive estimator robustly converges, and (ii) then, the parameter s_s is chosen sufficiently slow ($s_s > 0$) so that the cascade estimator functions with an adequate trade off between reconstruction rate and robustness.

4. ESTIMATOR IMPLEMENTATIONS

4.1 Tuning

The nominal detector and the passive estimator were tuned following the pole-placement geometric estimation tuning scheme presented in Alvarez and Lopez (1999). The output reference frequencies were set as $(\omega_1, \omega_2, \omega_3, \omega_4) = (1/2, 1/2, 2, 2)\omega_r$, where $\omega_r = 1/\tau_r$ min^{-1} is the characteristic time of the average reactor residence time $\tau_r = 200$ min. The damping factor was set as $\zeta = 0.71$, and the celerity parameter was set at $s = 10$ for both designs, meaning that their dynamics are set ten times faster than the natural output dynamics.

Following the tuning guidelines presented in the last subsection, the cascade estimator was tuned as follows: (i) the value $s_f = 10$ of the passive estimator was adopted, (ii) the damping factor $\zeta = 0.71$ was fixed, and (iii) the parameter s_s was gradually increased until a satisfactory functioning was attained at $s_s = 4$.

4.2 Functioning

To evaluate the estimator functioning, the estimator model was run with the following errors: -4% error in the activation energies of propagation, -20% error in the heat transfer coefficient, and no volume contraction (i.e., $\phi_1 = \phi_2 = \phi_3 = 1$ and $\phi_4 = \phi_5 = 0$).

The detector and passive estimator estimates are shown in Fig. 4. The detector estimates (thin continuous plots) exhibit a fast oscillation response with some offset. The passive estimator (discontinuous plots) has a behavior in the other way around: slow non-oscillatory convergence with larger offset. These results (Lopez and Alvarez, 2003) are in agreement with the conditioning assessment of the observability and passive innovation matrices presented in Fig. 3.

The cascade estimator functioning presented in Fig. 4, showing the estimates, has effectively achieved a better compromise between performance and robustness: the behavior retains features of both nominal and passive structures, so the motions are slightly oscillating (mainly for the composition), there are minor offsets, and fast convergence rates are attained.

7.CONCLUSIONS

The problem of the product quality and production rate inference has been addressed of a copolymer reactor, using on-line secondary measurements. Three different nonlinear estimation structures were considered: (a) the nominal detectability structure, that maximizes the reconstruction rate, (b) the passive estimation structure that maximizes the robustness, and (c) the proposed cascade estimation structure which superimposes a fast passive detector with a slow nominal detector, achieving a better compromise between performance (fast reconstruction rate) and robustness (tolerance to modeling error and error propagation). Invoking singular perturbation arguments, the cascade estimator convergence was established in terms of a cascade control like criterion: a fast passive gain with a sufficiently slow detectability gain.

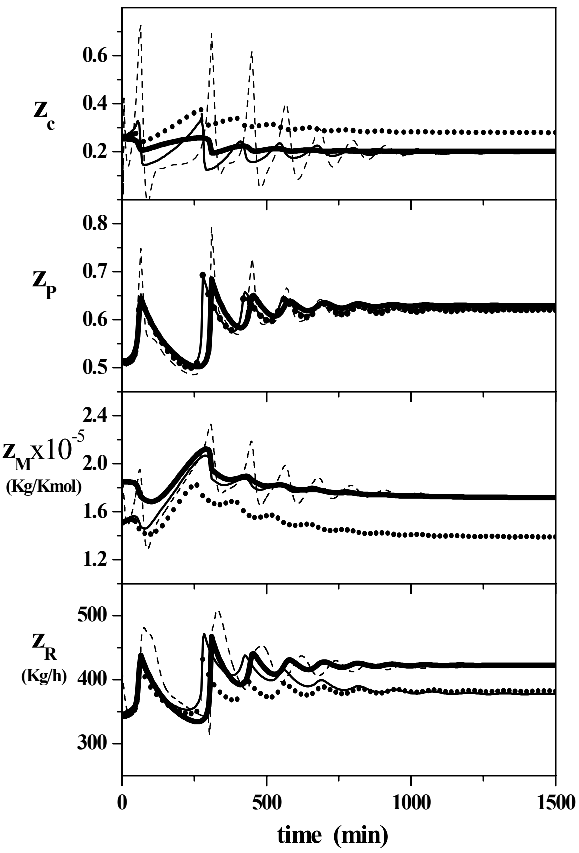

Fig. 4. Dynamic response of the reactor (▬▬▬), of the detector (— — —), of the passive estimator (·····), and of the cascade estimator (———).

REFERENCES

Alvarez, J. (2000). Nonlinear state estimation with robust convergence, *J. Proc. Control*, 10, 59.

Alvarez, J. and T. López (1999). Robust Dynamic State Estimation of Nonlinear Plants, *AIChE J.*, 45(1), 107.

Dimitratos, J., C. Georgakis, M. El-Aasser and A. Klein (1991). An Experimental Study of Adaptive Kalman Filtering in Emulsion Copolymerization. *Chem. Eng. Sci*., 46, 3203-3218.

Ellis, M.F., T.W. Taylor and K.F. Jensen (1994). On-line Molecular Weight Distribution Estimation and Control in Batch Polymerization Reactors. *AIChE J.*, 40, 445-462.

Hamer, J.W., T.A. Akramov and W.H. Ray (1981). The Dynamic Behavior of Continuos Polymerization Reactors - II. Nonisothermal Solution Homopolymer. and Copolymerization in a CSTR. *Chem. Eng. Sci.*, 36, 1897-1914.

Hermann, R. and A.J. Krener (1997). Nonlinear controllability and observability, *IEEE TAC AC*-22, 5.

Hernandez, H. and J. Alvarez (2003). Robust estimation of continuous nonlinear plants with discrete measurements, *J. Proc. Control*,13(1), 69

Lopez, T. (2000). Estimacion y control no lineal de reactores de copolimerizacion. *Ph. D. Thesis*, Universidad Autonoma Metropolitana, Mexico.

Lopez, T. and J. Alvarez (2003). On the effect of the estimation structure in the functioning of a nonlinear copolymer reactor estimator, submitted to the *J. Proc. Control*.

Lopez, T., S. Tronci, R. Baratti, and J. Alvarez (2002). State estimation in a catalytic reactor via a constructive approach, *Proc. IFAC World Cong*., Barcelona, Spain.

Lorimer, J.W. (1972). Refractive index increments of polymers in solution: 3. Dependence on concentration, *Polymer*, 13, 274.

Mutha, R. K., W.R. Cluett, and A. Penlidis (1997). On-line nonlinear model-based estimation and control of a polymer reactor, *AIChE J*., 43, 3042.

Kristic, M., I. Kanellapoulos and P. Kokotovic (1995). *Nonlinear and Adaptive Control Design*. Wiley, New York.

Padilla, S. and J. Alvarez (1997). Control of Continuous Solution Copolymerization Reactors. *AIChE J*., 43(2), 448.

Ray, W.H. (1986). Polymerization Reactor Control, *IEEE Control systems,* 6(4), 3.

Sepulchre, R., Jankovic, M. and Kokotovic, P.V. (1997). *Constructive Nonlinear Control*. Springer-Verlag, London

Sontag, E. D. (1990). *Mathematical control theory, Deterministic finite dimensional systems*. Springer-Verlag, New York.

Van Dooting, M., V.D. Rakotrapa, J.P. Gauthier and P. Hobbes (1992). Nonlinear Deterministic Observer for State *Estimation*: Application to a Continuous Free-Radical Polymerization Reactor, *Comp. Chem. Eng*. 16, 777.