INTERLACED ESTIMATOR-CONTROL DESIGN FOR CONTINUOUS EXOTHERMIC REACTORS WITH NON-MONOTONIC KINETICS

Jorge Diaz-Salgado * **Alexander Schaum** *
Jaime A. Moreno * **Jesus Alvarez** **

* *Instituto de Ingeniería, Universidad Nacional Autónoma de México (UNAM). Cd. Universitaria, 04510 México D.F.*
** *Universidad Autonoma Metropolitana-Iztapalapa Apdo. 55534, (UAM-I), 09340 México DF.*

Abstract: The problem of controlling continuous exothermic jacketed reactors with non-monotonic kinetics as well as temperature, level and flow measurements is addressed. The application of a constructive control procedure, with emphasis on the attainment of linearity, decentralization, robustness and model independency features, yields: (i) a control scheme with PI volume and cascade temperature loops, (ii) a material balance concentration controller driven by the integral actions of the temperature controller, and (iii) a closed-loop nonlocal stability criterion coupled with conventional-like tuning guidelines. The approach is tested with a representative example through simulations.

Keywords: Reactor Control, PI Controllers, Constructive Control

1. INTRODUCTION

An important class of chemical and biological materials are produced in continuous reactors with non-monotonic reaction rate (Elnashaie *et al.*, 1990; Lapidus *et al.*, 1977). In exothermic reactors, the interplay between heat generation-removal and non-monotonic kinetics manifests itself as strongly nonlinear behavior, with asymmetric input-output coupling, steady-state (SS) multiplicity, and parametric sensitivity (Aris, 1969). Operation at maximum production rate means lack of local observability about the nominal SS (Diaz-Salgado *et al.*, 2006). To overcome this obstacle for estimator-based control, the reactor can be operated at a reaction rate sufficiently below its maximum value, at the cost of less productivity. In industry (Shinskey, 1988), volume and cascade temperature linear PI loops are employed, and the concentration is regulated by adjusting the reactant dosage via supervisory or advisory control. Thus, the objective of a process-control design scheme is to attain a closed-loop operation with an adequate compromise between safety, operability, productivity, and quality in the light of investment operation costs. Hitherto, this problem has been addressed with a diversity of procedures (Smets *et al.*, 2002) that lack systematization and formal closed-loop stability assessments, and recently with an output-feedback nonlinear passive controller (Diaz-Salgado *et al*, 2006). In spite of its robustness oriented developement, the consideration of the las controller should rise complexity, reliability, maintenance and cost concerns among practitioners because: (i) the scheme is rather complex and model dependent, (ii) the volume and jacket temperature control components are not included, and (iii) a formal stability assessment is lacking. These considerations motivate the present study. In this work, employing the same robustness oriented approach, the reactor problem is addressed within a constructive control framework. The result is a measurement-driven (MD) control scheme with: (i) decentralized linear PI volume and cascade temperature loops, a ratio-type material-balance concentration controller, (ii) reduced model dependency, especially of the components that perform the stabilization task, and (iii) a nonlocal closed-loop robust stability criterion coupled with conventional-like tuning guidelines. The approach is illustrated with a representative example through simulations.

2. CONTROL PROBLEM

Consider a continuous exothermic jacketed reactor with non-monotonic reaction rate ($\rho_c := \partial_c \rho = 0$):

$$\dot{T} = \beta\rho(c,T) + \frac{q_e}{v}(T_e - T) - U(c,T)(T - T_j) := f_T \quad (1a)$$

$$\dot{T}_j = \alpha_j U(c,T)(T - T_j) + \alpha_q q_j (T_{je} - T_j) := f_j \quad (1b)$$

$$\dot{c} = -\rho(c,T) + \frac{q_e}{v}(c_e - c) := f_c, z_c = c,\ z_T = T \quad (1c)$$

$$\dot{v} = q_e - q := f_v, z_v = v,\ y_T = T,\ y_j = T_j,\ y_v = v \quad (1d)$$

$$\Omega = \{\mathbf{x} \in \mathtt{X} \mid \rho_c(c,T)\}, c^* = \kappa(T) \ni \rho_c[\kappa(T), T] = 0$$

The *states* ($\mathbf{x}$) are the reactant (dimensionless) concentration (c) , reactor temperature (T), jacket temperature (T_j), and reactor volume (v). The *control inputs* ($\mathbf{u}$) are the feed (q_e) and exit (q) flows and the coolant flow (q_j). The *regulated outputs* ($\mathbf{z}$) are the concentration (c), the temperature (T), and the volume (v). The *measured outputs* ($\mathbf{y}$) are the volume (v), and the reactor (T) and jacket (T_j) temperatures. The *measured inputs* ($\mathbf{d}$) are the reactor (T_e) and jacket (T_{je}) feed temperatures, and the feed concentration (c_e) is an unmeasured input. U (or $\alpha_j U$) is the heat transfer coefficient divided by the reactor (or cooling system) heat capacity, β is the adiabatic temperature rise (heat of reaction to heat capacity quotient), and α_q is the product of the coolant density by the specific heat capacity divided by the heat capacity of the cooling system. The reaction rate function has non-monotonic dependency on c, and is maximum at the curve Ω in the $c - T$ plane. A given nominal temperature $\bar{T}$ uniquely determines the concentration c^* for maximum rate, and the reactor system is not locally observable at Ω. In vector notation, system (1) becomes

$$\begin{aligned}
&\dot{\mathbf{x}} = f(\mathbf{x},\mathbf{u},\mathbf{d}),\ \mathbf{x}(0) = \mathbf{x}_0, \quad \mathbf{y} = C_y\mathbf{x}, \mathbf{z} = C_z\mathbf{x} \\
&\qquad f(\bar{\mathbf{x}},\bar{\mathbf{u}},\bar{\mathbf{d}}) = 0, \qquad \bar{\mathbf{y}} = C_y\bar{\mathbf{x}}, \qquad \bar{\mathbf{z}} = C_z\bar{\mathbf{x}} \\
&\mathbf{x} = [c, T, T_j, v]^T \in X, \quad \mathbf{y} = [T, T_j, v]^T \in Y \\
&\mathbf{z} = [c, T, v]^T \in Z, \quad \mathbf{d} = [T_e, T_{je}, c_e]^T \in D \\
&\mathbf{u} = [q_e, q, q_j]^T \in U
\end{aligned}$$

The definition of nonlocal stability that underlies our study is stated next. Consider a nonlinear system with time-varying exogenous input $d_e(t)$:

$$\dot{e} = f_e(e, d_e),\ e(0) = e_0,\ f_e(0,0) = 0$$

The steady-state $e = 0$ is input-to-state (IS) stable (Sontag, 2000) if there is a KL-class (increasing-decreasing) function α and a K-class (increasing) function γ so that

$$|e(t)| \le \alpha(|e_o|, t - t_o) + \gamma(||d_e(t)||), t \ge 0$$
$$||d_e(t)|| = sup|d_e(t)|, \quad t \ge 0$$

where α (or γ) bounds the transient (or asymptotic) response. The (necessary and sufficient) Lyapunov characterization of the IS stability property is given by (Sontag, 2000)

$$\alpha_1(|e|) \le V(e) \ \le \alpha_2(|e|),\ \dot{V} = -\ \alpha_3(|e|) + \alpha_4(||d_e||)$$

where V is a positive definite radially unbounded function and α_i is a K-class function. If the stability property holds for prescribed initial state, input, and state deviation sizes, the SS ($e = 0$) steady-state is said to be practically stable (Freeman *et al.*, 1996).

Our *problem* consists in designing a controller that, driven by the measurements $\mathbf{y}$, regulates the operation about a (possibly open-loop unstable) nominal SS $\bar{\mathbf{x}} = [e^* = \kappa(\bar{T}), \bar{T}]$ with maximum reaction rate. We are interested in: (i) a closed-loop robustly stable functioning, (ii) a systematic construction-tuning procedure, and (iii) the attainment, as much as possible, of linearity, decentralization, robustness and modeling independency features.

3. FEEDFORWARD (FF)-STATE-FEEDBACK (SF) CONTROL

Geometric Control. Regarded individually, the coolant flow-temperature input-output pair $q_j - z_T$ has relative degree (RD) equal to 2, the associated controller (q_j) requires the feed flow (q_e) control derivative, and consequently, the 3-input ($\mathbf{u}$) 3-output ($\mathbf{z}$) reactor system (1) does not have RD's, meaning that the FF-SF problem cannot be solved with static control. From the application of the dynamic extension procedure (Isidori, 1995), the next proposition follows [the function $f(x_1, \ldots, x_n)$ is said to be χ_i-monotonic if $\partial_{x_i} f$ is of one sign]. With the dynamic extension $(\dot{q}, \dot{q}_e) = (\upsilon_q, \upsilon_{q_e})$, the reactor has relative degree (rd) vector κ (2) if and only if conditions (3) are met, in a compact set about $\bar{\mathbf{x}}$:

$$\kappa = (\kappa_v, \kappa_e, \kappa_T) = (2, 2, 2) \quad (2)$$

$$c \ne 1, T_{j_e} \ne T_j, \quad f_T : T_j - monotonic \quad (3)$$

Conditions (3) are always met because they say that: (i) the reactant is part of the reacting mixture, (ii) there is reactor-jacket heat exchange, and (iii) the heat exchange rate is uniquely determined by the jacket temperature. The related zero-dynamics (ZD) are trivially given by the nominal SS $\bar{\mathbf{x}}$. From the enforcement of the linear, non interactive, pole assignable (LNPA) output regulation dynamics (4), the *nonlinear geometric dynamic FF-SF controller* of form (5) follows.

$$\ddot{e}_a + \zeta_a\omega_a\dot{e}_a + \omega_a^2 e_a = 0, \quad a = v, c, T \quad (4)$$

$$(\dot{q}, \dot{q}_e) = \mu_q^g(v, c, T, T_j, q, q_e, T_e) \quad (5)$$
$$q_j = \mu_j^g(v, c, T, T_j, q, q_e, T_e, T_{j_e}, \dot{T}_e)$$

The IS stability of the resulting closed-loop system is a consequence of the IS stability of the LNPA (4). This controller: (i) has two dynamic components and a static one, (ii) has a dynamic-to-static component cascade interconnection, (iii) requires the derivatives of the exogenous input T_e, and (iv) all components depend on the entire state-input pair $\mathbf{x} - \mathbf{u}$.

Passive Control. From a constructive control perspective (Krstic *et al.*, 1995) robustness is a major drawback of controller (5), because it is not underlain by a structure with all the relative degrees equal or less than 1. To remove this obstacle, let us redesign the controller with passivation by backstepping (Krstic *et al.*, 1995). Introduce the Lyapunov function (6) (where T_j^* is the jacket temperature virtual control), enforce the dissipation rate (7)

$$V_p = V_c^p + V_T^p + V_v^p, \qquad V_c^p = e_c^2/2 \quad (6)$$
$$V_T^p = (e_T^2 + e_j^2)/2, \qquad V_v^p = e_v^2/2$$
$$e_c = c - \bar{c},\ \mathrm{e}_T = T - \bar{T}, e_j = T_j - T_j^*,\ \mathrm{e}_v = v - \bar{v}$$
$$\dot{V}_p = -k_c e_c^2 - k_T e_T^2 - k_j e_j^2 - k_v e_v^2 < 0 \quad (7)$$

and obtain the *nonlinear static stabilizing FF-SF passive controller*

$$q_e = v[-k_c(c - \bar{c}) + \rho(c, T)]/\,(c_e - c) \quad (8a)$$
$$q = -k_v(v - \bar{v}) + q_e \quad (8b)$$
$$q_j = \mu_j(c, T, v, c_e, T_e, q, q_e) \quad (8c)$$

$\mu_j(c, T, T_j^*, v, c_e, T_e, q, q_e, \dot{T}_j^*) = \frac{\dot{T}_j^* - k_j(T_j - T_j^*) - \alpha_j U(T - T_j)}{\alpha_q(T_{je} - T_j)}$
$T_j^* = T + \left[-k_T(T - \bar{T}) - \beta\rho(c, T) - \frac{q_e}{v}(T_e - T)\right]/U$ $\dot{T}_j^* = \frac{1}{U}\left[-k_T\dot{T} - \beta\left(\rho_c\dot{c} + \rho_T\dot{T}\right)\right] - \frac{q_e}{U}\left(\frac{(\dot{T}_e - \dot{T})v - (q_e - q)(T_e - T)}{v^2}\right)$
$\dot{T} = f_T(c, T, v, T_j, T_e, q_e)$

The closed-loop robustly stable behavior of this controller constitutes the recovery target for the output feedback (OF) control design on the next section.

4. OUTPUT FEEDBACK (OF) CONTROL

In this section, the behavior of the exact model-based passive nonlinear controller (8) is recovered via an interlaced control-observer design with emphasis on the attainment of linearity, decentralization, and model independency features.

4.1 OF Control with EKF

Since the reactor is not locally observable at the curve Ω, a nonlinear high-gain Luenberger observer cannot be applied, and therefore an EKF (9) for the reactor system (1) is set, and its combination with the nonlinear FF-SF passive controller (8) yields the *EKF-based OF controller.*

$$\dot{\hat{c}} = -\rho(\hat{c}, \hat{T}) + [q_e(c_e - \hat{c})]/y_v + \frac{\sigma_{12}}{r_{11}}\left(y_T - \hat{T}\right) \quad (9a)$$
$$\dot{\hat{T}} = \beta\rho(\hat{c}, \hat{T}) + [q_e(T_e - \hat{T})]/y_v - U(\hat{T} - T_j)$$
$$+\frac{\sigma_{22}}{r_{11}}\left(y_T - \hat{T}\right) \quad (9b)$$
$$\dot{\sigma}_{11} = 2\left[(-\rho_c(\hat{c}, \hat{T}) + \frac{q_e}{y_v})\sigma_{11} - \rho_T(\hat{c}, \hat{T})\sigma_{12}\right]$$
$$+q_{11} - \frac{\sigma_{12}^2}{r_{11}}, \qquad \rho_T = \partial_T\rho \quad (9c)$$
$$\dot{\sigma}_{22} = 2\left[\beta\rho_c(\hat{c}, \hat{T})\sigma_{12} + (\beta\rho_T(\hat{c}, \hat{T}) - \frac{q_e}{y_v} - U)\sigma_{22}\right]$$
$$+q_{22} - \frac{\sigma_{22}^2}{r_{11}} \quad (9d)$$
$$\dot{\sigma}_{12} = \beta\sigma\rho_c(\hat{c}, \hat{T})_{11} + [-\rho_c(\hat{c}, \hat{T}) + \frac{q_e}{y_v} + \beta\rho_T(\hat{c}, \hat{T})$$
$$-\frac{q_e}{y_v} - U]\sigma_{12} - \rho_T(\hat{c}, \hat{T})\sigma_{22} - \frac{\sigma_{12}\sigma_{22}}{r_{11}} + q_{21} (9e)$$

$$q_e = y_v(-k_c(\hat{c} - \bar{c})) + \rho(\hat{c}, \hat{T}, p)/\,(c_e - \hat{c}) \quad (10a)$$
$$q = -k_v(y_v - \bar{v}) + q_e \quad (10b)$$
$$q_j = \mu_j(\hat{c}, \hat{T}, y_j, y_v, c_e, T_e, q, q_e) \quad (10c)$$

where σ_{nn} are the elements of the error covariance matrix. This controller: (i) consists of 5 ordinary differential equations (ODE's) and 5 algebraic ones (AE's), and (ii) needs the detailed model (1).

4.2 Interlaced estimation-control design

From an industrial control perspective, the OF controller (9,10) is rather complex and model dependent. In this section, the controller is redesigned to overcome this drawbacks.

Control Model. On the basis of its relative degree-detectability structure (Alvarez *et al.*, 2007) let us rewrite the *reactor system* (1) in the linear dynamic-nonlinear static form

$$\dot{c} = -r + q_e(c_e - c)/v \quad (11a)$$
$$\dot{T} = a_T T_j + b_T, \qquad y_T = T \quad (11b)$$
$$\dot{T}_j = a_j q_j + b_j, \qquad y_j = T_j \quad (11c)$$
$$\dot{v} = a_v q + b_v, \qquad y_v = v \quad (11d)$$
$$r = [b_T - \frac{b_v}{v}(T_e - y_T) + \frac{1}{\alpha_j}(b_j + \quad (11e)$$
$$-\alpha_q q_j(T_{je} - T_j) + a_j q_j) + a_T T_j]/\beta (11f)$$
$$a_T \approx \bar{U}, a_j \approx \bar{\alpha}_j(\bar{T}_{je} - \bar{T}_j), a_v \approx -1 \quad (11g)$$

$$b_T = \Theta_T(c, T, T_j, v, T_e, q_e) = \beta\rho(c, T) + (q_e/v)(T_e - T) - U(T - T_j) - a_T T_j \quad (11h)$$

$$b_j = \Theta_j(T, T_j, T_{je}, q_j) = U\alpha_j(T - T_j) + q_j\alpha_q(T_{je} - T_j) - a_j q_j \quad (11i)$$

$$b_v = \Theta_v(q_e) = q_e \quad (11j)$$

where $rd(T_j, y_T) = rd(q_j, T_j) = rd(q, y_v) = rd(b_T, y_T) = rd(b_j, y_j) = rd(b_v, y_v) = 1$

the unknown input (b_j, b_v, b_T) is instantaneously observable because it is timewise determined by $(y, \dot{y})$, implying that the concentration can be reconstructed by integrating its mass balance driven by (y, b). Moreover, the reaction rate value r can be on-line reconstructed without needing the reaction rate function-heat transfer pair, in agreement with the calorimetric estimation approach (Alvarez-Ramirez *et al.*, 2002).

Estimator. From standard reduced-order observation techniques (Stefani *et al.*, 1994) in conjunction with the heat balance-based expression of r as function of (b_j, b_v, b_T), the next estimator follows

$$\dot{\chi}_\iota = -\omega_\iota\chi_\iota - \omega_\iota^2 y_\iota - \omega_\iota a_\iota u_\iota, \chi_\iota(0) = -\omega_\iota y_\iota(0) \quad (12)$$

$$\hat{b}_\iota = \chi_\iota + \omega_\iota y_\iota \qquad \iota = v, T, j$$

$$\hat{r} = [\chi_T + \omega_T y_T - \frac{q_e}{v}(T_e - y_T) + \frac{1}{\alpha_j}(\chi_j + \omega_j y_j - \alpha_q q_j(T_{je} - y_j) + a_j q_j) + a_T y_j]/\beta \quad (13)$$

Regard the reaction rate estimate (13) as a *virtual measurement* for the concentration dynamics and write the corresponding EKF

$$\dot{\hat{c}} = -\hat{r} + \frac{q_e}{v}(c_e - \hat{c}) + s\rho_c(\hat{c}, \hat{T}, p)\left[\hat{r} - \rho(\hat{c}, \hat{T}, p)\right] \quad (14a)$$

$$\dot{s} = -2sq_e/v + \nu - \rho_c^2(\hat{c}, \hat{T}, p)s^2,\ s(0) = s_0 \quad (14b)$$

$$s = \sigma/q_r, \quad \nu = q_c/q_r$$

where q_c (or q_r) is the model (or measurement) noise intensity, σ is the concentration error covariance, and $s\rho_c$ is the estimator gain, and ν is an adjustable (speed) parameter.

Measurement-driven controller. The combination of the last estimator (12,13,14) with the nonlinear FF-SF passive controller (8) yields the *constructive output-feedback controller*

- Temperature controller (15a)

$$\dot{\chi}_T = -\omega_T\chi_T - \omega_T^2 y_T - \omega_T a_T T_j^*$$

$$Tj^* = \left(-k_T(y_T - \bar{T}) - \chi_T - \omega_T y_T\right)/(a_T)$$

$$\dot{\chi}_j = -\omega_j\chi_j - \omega_j^2 y_j - \omega_j a_j q_j$$

$$q_j = \left(\dot{T}_j^* - k_j(y_j - Tj^*) - \chi_j - \omega_j y_j\right)/(a_j)$$

$$\dot{T}_j^* = -k_T T_j - \frac{k_T}{a_T}\chi_T - \frac{k_T\omega_T}{a_T}T$$

- Volume controller (15b)

$$\dot{\chi}_v = -\omega_v\chi_v - \omega_v^2 y_v - \omega_v a_v q$$

$$q = (-k_v(y_v - \bar{v}) - \chi_v - \omega_v y_v)/(a_v)$$

- Concentration controller (15c)

$$q_e = \frac{y_v\left(-k_c(\hat{c} - \bar{c}) + \hat{r}\right)}{(c_e - \hat{c})}$$

$$\hat{r} = [\chi_T + \omega_T y_T - \frac{q_e}{v}(T_e - y_T) + \frac{1}{\alpha_j}(\chi_j + \omega_j y_j - \alpha_q q_j(T_{je} - y_j) + a_j q_j) + a_T y_j]/\beta$$

$$\dot{\hat{c}} = -\hat{r} + \frac{q_e}{y_v}(c_e - \hat{c}) + s\rho_c(\hat{c}, T, p)\left[\hat{r} - \rho(\hat{c}, T, p)\right]$$

$$\dot{s} = -2sq_e/y_v + \nu - \rho_c^2(\hat{c}, T, p)s^2$$

In classical PI form, the temperature (15a) and volume (15b) controllers are written as follows:

$$u_\iota = \frac{\dot{\bar{y}}_\iota}{a_\iota} - \kappa_\iota\left[(y_\iota - \bar{y}_\iota) + \frac{1}{\tau_\iota}\int_0^t (y_\iota(\sigma) - \bar{y}_\iota(\sigma))\,d\sigma\right]$$

$$\kappa_\iota = (\omega_\iota + k_\iota)/a_\iota, \qquad \tau_\iota = \omega_\iota^{-1} + k_\iota^{-1}$$

This controller (15) consists of 5 ODE's and 6 AE's. The concentration component: (i) is a material balance controller driven by the information generated in the temperature controller, and (ii) only needs a tendency reaction rate function to set the innovation. The functioning of the PI volume and temperature components is independent of the concentration controller.

4.3 Closed-loop stability and tuning

In a way that parallels the closed-loop stability proof of a polymer reactor with PI inventory control (Alvarez *et al.*, 2007), recall the LFs (6) of the nonlinear FF-SF passive controller (8) and of the open-loop estimator (12), and apply Lyapunov's direct method to draw the next proposition.

Proposition 1. (Sketch of Proof in Appendix A). Consider the reactor (1) with the proposed OF controller (15). The resulting closed-loop system is IS-stable if: (i) the gain pair (k_c, ϖ) of the unmeasured output $(z_c = c)$ is chosen according with (16a), and (ii) the gains of the primary (k_v, k_T) and secondary (k_j) control and estimator $(\omega_v,\ \omega_T,\ \omega_j)$ components are tuned so that the dynamic separation conditions (16b, 16c) are met:

$$k_c = \varpi q/y_v, \varpi \in (\varpi^-, \varpi^+), \varpi^\pm = 3 \pm 2\sqrt{2} \quad (16a)$$

$$k_p^- < k_p < k_p^+ = \gamma_p^+(\omega), k_j < k_j^+(\omega) \quad (16b)$$

$$\omega = min(\omega_v, \omega_T, \omega_j) < \omega^+ \qquad \square \quad (16c)$$

Conditions (16a) ensure the stability of the (unmeasured) state concentration dynamics, regarded individually. In conditions (16b,16c): (i) ω^+ is an upper gain limit imposed by the high-frequency not modeled dynamics, (ii) k_p^- is a lower primary gain limit due to the open-loop reactor

Table 1. Steady states

$k = e^{25}, \gamma = 1e4, \sigma = 3, U = c_e = \alpha_q = 1, T_e = T_j = 370$			
$\beta = 200, \alpha_j = 10, q_e = q = 0.989, q_j = 8.685, T_{je} = 293$			
steady-state	S_E	U	S_I
concentration [mol/L]	0.998	0.333	0.017
temperature [K]	345.54	436.07	479.07
jacket temperature [K]	321.12	369.57	392.58
volume [L]	1.0	1.0	1.0
local condition	stable	unstable	stable

instability, and (iii) γ_p^+ (or γ_j^+) is an isotonic function that sets an upper limit k_j^+ (or k_p^+) for the secondary (or primary) gain, depending on the (faster) estimation (ω) [or secondary (k_j)] gain. Thus, the choice of gains affects and is affected by the sizes of the prescribed (or to be compromised) initial state, exogenous input, and model parameter disturbance sizes, in agreement with the practical stability framework (Freeman *et al.*, 1996). From the preceeding stability analysis, the conventional-like tuning guidelines follow. (i) Set: the unmeasured output gains at their nominal values of their associated dilution rates ($\varpi = 1$), the control gains at the nominal inverse residence time ($k_v = k_T = k_j = \bar{q}/\bar{v}$), and the estimator gains about three times faster ($\omega_v = \omega_T = \omega_j = 3\bar{q}/\bar{v}$). (ii) Increase ω up to its ultimate value ω_u (where oscillatory response is obtained), and back-off so that satisfactory behavior is attained ($\omega \approx \omega_u/3$). (iii) Increase the volume gain k_v up to its ultimate value k_{vu}, and back off ($\approx k_v \leq k_{vu}/3$) for adequate response. Repeat the procedure for the secondary temperature gain k_j ($\approx k_j \leq k_{ju}/3$). (iv) Increase the temperature gain k_T up to its ultimate value k_{Tu}, and back-off until an adequate response is attained. (v) Apply the same increase-plus-back-off procedure to the unmeasured output gain ϖ, in the understanding that it cannot be larger than two to four times the reactor dilution rate (Alvarez *et al.*, 2007). (vi) If necessary, adjust the volume and temperature estimator gains.

5. APPLICATION EXAMPLE

The model functions and parameter values (listed in Table 1) were adapted from an experimental catalytic reactor (Baratti *et al.*, 2002). The reaction rate function is given by:

$$\rho(c, T, p) = (cke^{-\left(\frac{\gamma}{T}\right)})/\left(1 + \sigma c\right)^2 \, [mol/L \cdot \mathrm{min}]$$

The reactor has three SS's (listed in Table 1), two of them corresponding to extinction (S_E) and ignition (S_I) stable operations, and one being unstable (U). To subject the controller to a severe test the reactor must be operated about the unstable SS with maximum reaction rate. The initial conditions for closed-loop testing were about the unstable steady-state: $x(0) = [0.2, 430, 365, 0.9]^T$

Tuning. For the constructive controller (15), the application of its tuning guidelines yielded: $\omega_v = 50$ min^{-1}, $\omega_j = 20, \omega_T = 50$, $k_v = 3, k_j = 6, k_T = 3, \varpi = 1 = \nu = 1 \hat{c}(0) = 0.25, \hat{T} = 440, \sigma(0) = 0, \chi_j(0) = -\omega_j Tjo, \chi_T o = -\omega_T To, \chi_v o = -\omega_v v_0$

The EKF-based controller (9,10) was tuned with: $q_{11} = 7.590 \times 10^{-3}, q_{22} = 6.006 \times 10^{-7}, q_{21} = 0, r_{11} = 2.376 \times 10^{-7}, \hat{c}(0) = 0.25, \hat{T}(0) = 440, \sigma_{11}(0) = \sigma_{12}(0) = \sigma_{22}(0) = 0$

Nominal Behavior. With the actual parameter values, the (detailed model-based) EKF-nonlinear (9,10) and (simplified model-based) proposed OF (15) controllers were applied to the reactor, and the result behaviors are presented in Fig. 1, yielding that both controllers: (i) stabilize the reactor and exhibited the same overall functioning, and (ii) recover the behavior (not shown) of the exact model-based nonlinear passive controller (8).

Robust Behavior. The EKF-nonlinear (9,10) and proposed OF (15) controllers were run with typical parameter errors: −9.5% in the pre-exponential factor k, −0.5% in the adsorption constant σ and −6.6% in the activation energy γ, in the understanding that the highly nonlinear and uncertain rate-heat exchange function pair is not needed by the proposed control scheme. The corresponding closed-loop responses are presented in Fig. 2, showing that: (i) the proposed OF controller (15) outperforms its EKF-based (9,10) counterpart, (ii) the behavior of the constructive controller with parameter errors is very similar to the one (see Fig. 1) of its errorless counterpart. While the tuning of the constructive controller was a rather straightforward task, the tuning of the EKF-nonlinear passive controller require some effort.

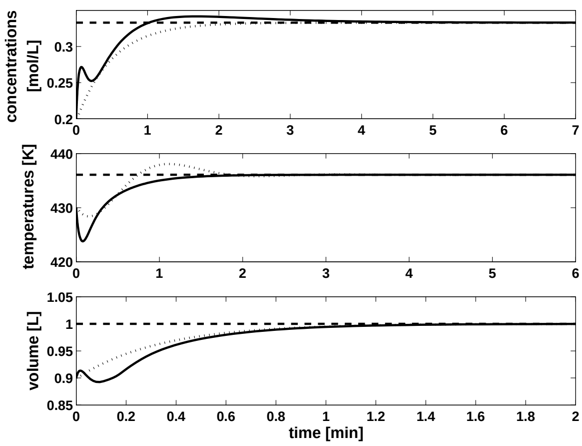

Fig. 1. Nominal behavior with (9,10) EKF-nonlinear (..) and (15) constructive (-) controllers.

6. CONCLUSIONS

A constructive robust MD control design methodology for continuous reactors with non-monotonic

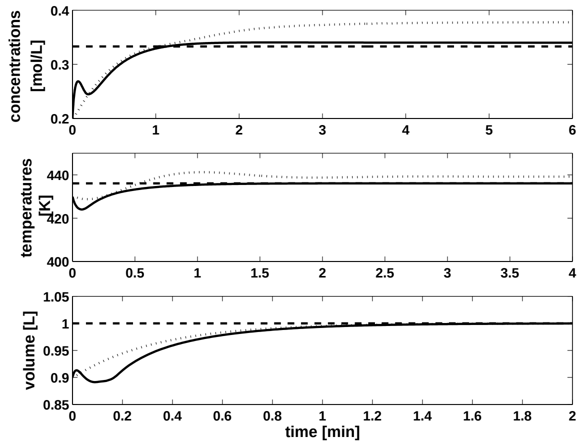

Fig. 2. Robust behavior with (9,10) EKF-nonlinear (..) and (15) constructive (-) controllers.

kinetics as well as flow and temperature measurements has been presented. The application of a Lyapunov interlaced estimator-control design yielded an OF control scheme with: (i) linear-decentralized PI volume and control components, (ii) a ratio-type material-balance concentration controller that exploits the information contained in the integral actions of the temperature controller, (iii) a systematic construction procedure, and (iv) a closed-loop nonlinear-nonlocal stability criteria coupled with simple tuning guidelines. The proposed controller (15): is considerably simpler and less model dependent than its EKF-based nonlinear control counterpart (9,10), and amounts to a scheme with decentralized components that resembles the ones employed in industrial reactors. An open-loop unstable reactor was addressed with numerical simulations.

Appendix A. CLOSED-LOOP DYNAMICS

The application of the constructive controller (15) to the reactor (1) yields the *closed-loop dynamics*

$$\dot{e}_c = -k_c e_c + q_c(c, T, T_j, v, T_e, T_{je}, c_e, s, b_T, b_j; \epsilon_T, \epsilon_j, \epsilon_c) \quad \text{(A.1a)}$$

$$\dot{e}_T = -k_T e_T + q_T(T, b_T; \epsilon_T) \quad \text{(A.1b)}$$

$$\dot{e}_j = -k_j e_j + q_j(T, T_j, b_T, b_j; \epsilon_T, \epsilon_j) \quad \text{(A.1c)}$$

$$\dot{e}_v = -k_v e_v + q_v(v, b_v; \epsilon_v) \quad \text{(A.1d)}$$

$$\dot{\epsilon}_T = -\omega_T \epsilon_T + (\ddot{T} - a_T \dot{T}_j) \quad \text{(A.1e)}$$

$$\dot{\epsilon}_j = -\omega_j \epsilon_j + (\ddot{T}_j - a_j \dot{q}_j) \quad \text{(A.1f)}$$

$$\dot{\epsilon}_v = -\omega_v \epsilon_v + (\ddot{v} - a_v \dot{q}) \quad \text{(A.1g)}$$

$$\dot{\epsilon}_c = -k_c \epsilon_c - s\rho_c(\hat{c}, T)\left[\hat{r} - \rho(\hat{c}, T)\right] \quad \text{(A.1h)}$$

$$\dot{s} = \frac{-2s}{c_e - \hat{c}}\left[-k_c(e_c + \epsilon_c) + \hat{r}\right] + \nu + -s^2\rho_c^2(\hat{c}, T) \quad \text{(A.1i)}$$

where: $e_c = c - \bar{c}, e_T = T - \bar{T}, e_v = v - \bar{v}, e_j = T_j - T_j^*, \epsilon_c = c - \hat{c}, \epsilon_T = b_T - \hat{b}_T, \epsilon_j = b_j - \hat{b}_j, \epsilon_v = b_v - \hat{b}_v$.

Proof of Proposition 1 Recall the LF (6), introduce the redesigned LF

$$V = V_p + \hat{V}, \quad \hat{V} = \hat{V}_v + \hat{V}_c + \hat{V}_T + \hat{V}_s, \quad \hat{V}_s = s^2/2$$
$$\hat{V}_v = \epsilon_v^2/2, \quad \hat{V}_c = c^2/2, \quad \hat{V}_T = (\epsilon_T^2 + \epsilon_j^2)/2$$

take its derivative along the closed-loop reactor (1) with the estimation error dynamics (A.1), and obtain the dissipation rate

$\dot{V} = -\alpha(e, \epsilon, \delta) + \tau(e, \epsilon, \delta, \dot{\delta}), \ \alpha(e, \epsilon, \delta) \geq 0, \ \tau(0,0,0,0) = 0$ where:

$$\begin{aligned}
\alpha &= k_v e_v^2 + \omega_v \epsilon_v^2 + k_T e_T^2 + \omega_T \epsilon_T^2 + k_j e_j^2 + \omega_j \epsilon_j^2 + s^2[s\rho_c^2 + 2\rho/(c_e - \hat{c})] \\
\delta &= (\delta_d, \dot{\delta}_d), \quad \delta_d = d - \bar{d}, \quad \lambda_q = q/v \\
\tau &= -(\dot{b}_v + e_v)\epsilon_v - (\dot{b}_T + e_T)\epsilon_T + s\nu - (\dot{b}_j + e_j)\epsilon_j + 2[s^2/(c_e - \hat{c})][k_c(e_c + \epsilon_c) - \tilde{r}] \\
\omega(x, y, \varpi) &= \varpi x^2 + (\varpi - 1)xy + y^2 > 0
\end{aligned}$$

Set the equation (A.2a), recall the closed-loop IS stability (7) with the passive controller (8), conclude the existence of a local asymptotic gain γ (A.2b), draw the dissipation rate inequality (A.3)

$$\alpha(e, \epsilon, \delta) = \tau(e, \epsilon, \delta, \dot{\delta}) \Rightarrow \left| \left(e', \epsilon'\right)' \right| = \gamma\left(\| \delta', \dot{\delta}' \|\right) \quad \text{(A.2)}$$

$$\dot{V} \leq 0 \forall \left| \left(e', \epsilon'\right)' \right| \geq \gamma(\| \delta(t) \|) \quad \text{(A.3)}$$

and conclude that the closed-loop reactor dynamics (A.1) is IS stable if the gains are chosen according to (16a,16b,16c). *QED*

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