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CONTROL OF CONTINUOUS REACTORS WITH NON-MONOTONIC REACTION RATE

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Abstract: In this paper, the problem of controlling a (possibly open-loop unstable) continuous exothermic chemical reactor with non-monotonic reaction rate, maximum production rate specification, and temperature measurements is addressed. The problem difficulty resides in the lack of reactor local observability at the nominal steady-state. A nonlocal constructive design approach leads to a passivated control scheme with linearity, decentralization and reduced model dependency features as well as nonlocal closed-loop behavior. The resulting control scheme resembles industrial type components: a linear PI cascade temperature controller, and a ratio inventory-based feedforward concentration controller. The approach is tested with a typical case example through numerical simulations.

Keywords: Reactor Control, Process Control.

1. INTRODUCTION

Reactors with non-monotonic kinetic rate dependency on concentration constitute an important class of reactors (Lapidus, 1977; Elnashaie, et al., 1990). These reactors may exhibit strongly nonlinear behavior, like steady-state multiplicity, limit cycling and parametric sensitivity. To obtain the maximum product yield, these reactors must be operated at a steady-state with maximum reaction rate, a concentration that is not locally observable from a temperature measurement. From a local control design viewpoint, this lack of observability means that, in spite of being able to control the temperature, it is not possible to know if the reactor concentration is in the isotonic or antitonic branch of the reaction rate function. This problem has been tackled by choosing a nominal concentration sufficiently below the one of the maximum rate (Smets, et al., 2002). So that locally: the reaction rate becomes monotonic, the steady-state is observable, and the concentration can be estimated and/or controlled. However, in the theoretical systems estimation literature is well known that lack of local (linear) observability does not necessarily imply lack of nonlocal (nonlinear) observability (Hermann and Krener, 1977), and this motivates the question addressed in the present work; on whether it is possible to nonlocally control a continuos reactor with non-monotonic reaction rate about a prescribed (possibly open-loop unstable) steady-state with maximum reaction rate. On the other hand, in a recent control study for an exothermic polymer reactor with monotonic reaction rates, the combination of feedfordward, passivity and observability ideas yielded an output feedback cascade

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controller with (Gonzalez and Alvarez, 2005): (i) linearity, decentralization and model independency features, (ii) industrial-like (linear PI, ratio and inventory) components, and (iii) behavior recovery of an exact model-based nonlinear state-feedback (SF) passivated controller. In this paper, the problem of controlling a (possibly open-loop unstable) continuous exothermic chemical reactor with non-monotonic reaction rate, maximum production rate specification, temperature measurements, and heat exchange and reactant dosage rate as manipulated variables is addressed. Having as point of departure the above discussed PI-inventory reactor control scheme, the combination nonlocal of passivity, observability and stability notions within robustness-oriented constructive control framework yields a measurement-driven dynamic control scheme that non-locally stabilizes the non-monotonic rate reactor about a steady state with maximum reaction rate. The resulting controller has two parts that resemble industrial conventional control components: (i) a PI temperature controller with a measurement noise filter, and (ii) a feedforward-like ratio controller for the reactant dosage rate. The proposed approach is tested with a case example through numerical simulations.

2. CONTROL PROBLEM

Consider a continuous chemical reactor where an exothermic reaction takes place, the volume is kept constant with suitable level control loop, heat exchange is enabled via a cooling jacket, by manipulating its temperature T_j, in the understanding that T_j is the set-point signal to drive a secondary control loop in a cascade configuration. Since the secondary temperature control loop design can be performed with existing techniques (Alvarez-Ramirez, et al., 2002; Gonzalez and Alvarez, 2005), here we will circumscribe to address the design of the primary temperature controller, in coordination with a composition regulation component. From standard mass and energy conservation arguments the reactor model is given by (Lapidus, 1977):

$$\begin{aligned}\dot{c} &= -\rho(c,T,p) + \theta(c_e - c)\\ \dot{T} &= \beta\rho(c,T,p) + \theta(T_e - T) - \upsilon(T - T_j)\\ y &= T, z_c = c, z_T = T, d_T = T_e, d_c = c_e\end{aligned} \quad (1)$$

Where c is the reactant dimensionless concentration T is the reactor temperature, T_j is the jacket temperature, θ is the dilution rate, υ is the heat transfer coefficient, and β is the adiabatic temperature rise (i.e., the heat of reaction divided by the reactor heat capacity). The *states* are the concentration c and the temperature T. The *control inputs* are the dilution rate θ and the jacket temperature T_j. The *regulated outputs* (z_c and z_T) are the concentration c and the temperature T. The *measured output* (y) is the temperature T. In other words, only one (the temperature) of the two regulated outputs is measured. The exogenous load disturbance inputs (d_T and d_c) are the measured feed temperature T_e and the unmeasured feed concentration c_e.

The strictly positive scalar function $\rho(c,T,p)$ describes the non-monotonic kinetic rate dependency on c and T, p is a parameter vector, and $\rho(c,T,p)$ has a maximum in the curve

$$\Omega = (c,T) \mid \frac{\partial\rho(c,T,p)}{\partial c} := \rho_c(c,T,p) = 0 \quad (2)$$

implying that the pair (T,p) uniquely determines a concentration value c^* where the reaction rate is maximum, this is,

$$c^* = \kappa(T,p) \ni \rho_c[\kappa(T,p),T,p] = 0$$

The reactor must operate about a (possibly open loop unstable) steady-state $\bar{x} = (\bar{c},\bar{T})^T$, and the nominal concentration $\bar{c}$ must yield the maximum reaction rate at $\bar{T}$, according to the steady-state expressions

$$\begin{aligned}0 &= -\rho(\bar{c},\bar{T},p) + \theta(\bar{c}_e - \bar{c}),\ \ \rho_c(\bar{c},\bar{T},p) = 0\\ 0 &= \beta\rho(\bar{c},\bar{T},p) + \theta(\bar{T}_e - \bar{T}) - \upsilon(\bar{T} - \bar{T}_j)\end{aligned} \quad (3)$$

where $\bar{c}_e$(or $\bar{T}_e$) is the nominal feed concentration (or temperature). In compact vector notation, the reactor (1) is written as follows

$$\dot{x} = f(x,d,u,p), \quad y = c_y x, \quad z = x$$

where
$x = [c,T]^T, d = [c_e,T_e]^T, c_y = [0,1], u = [\theta,T_j]$.

The controllability ($\mathcal{C}$) and observability ($\mathcal{O}$) matrix ranks of the linear reactor approximation about the prescribed steady-state ($\bar{x}$) are:

$$rank[\mathcal{C}] = 2 \Leftrightarrow \upsilon \neq 0, \bar{c}_e \neq \bar{c}\ ;\ \ \mathcal{C} = [B, AB]$$
$$rank[\mathcal{O}] = 2 \Leftrightarrow \rho_c(c,T,p) \neq 0\ ;\ \ \mathcal{O} = [c_y, c_y A]^T$$

where $A = f_x(\bar{x},\bar{d},\bar{u},p)$, $B = f_u(\bar{x},\bar{d},\bar{u},p)$.

Observe that: (i) at $\bar{x}$ the linear reactor approximation is controllable but not observable, (ii) when $x \neq \bar{x}$ the linear approximation is controllable and observable, and (iii) nowhere the reactor is nonlinearly instantaneously observable (Hermann and Krener, 1977; Alvarez, 2000) because, given $(T,\dot{T},T_j,T_e)$ the heat equation $\rho(c,T,p) = [\dot{T} - \theta(T_e - T) - \upsilon(T - T_j)]/\beta$ admits two concentration solutions. This signifies that a nonlinear high-gain Luenberguer observer cannot be employed (Zeitz, 1987), because the related observability matrix is singular at the curve Ω (2). Technically speaking, our problem is the following: given a prescribed steady-state operation (3), that is optimal in the sense that maximizes the production rate at $\bar{T}$, design an output-feedback

controller that, driven by measured output (y) and input (d_T) temperature measurements (without measuring the concentration), manipulates the dilution rate (θ) and the jacket temperature (T_j) to maintain the concentration (c) and temperature (T) outputs about their prescribed (possibly open loop unstable) steady-state values. In particular, we are interested in drawing a control design that: (i) is robust with respect to modeling and measurement uncertainties, and (ii) yields a robust closed-loop behavior with a suitable tuning scheme.

3. CONTROLLER CONSTRUCTION

3.1 State-feedback controller

For the moment, assume the *state* x, the *exogenous input* d, the model function, and the model parameters are known. Enforce the prescribed regulated output error dynamics

$$\dot{e}_c = -k_c e_c, \quad e_c = c - \bar{c} \tag{4}$$
$$\dot{e}_T = -k_T e_T, \quad e_T = T - \bar{T}$$

combine (4) with (1), and obtain the SF static controller

$$\theta = [-k_c(c-\bar{c}) + \rho(c,T,p)]/[c_e - c] \tag{5}$$
$$T_j = T + [-k_T(T-\bar{T}) - \beta\rho(c,T,p) - \theta(T_e - T)]/\upsilon$$

which is passive because it is underlain by a model (1) with relative degree pair $(1,1)$, and without zero-dynamics.

3.2 Output feedback controller

Given that the temperature pair (T, T_e) is measured, the feed concentration (c_e) is nearly constant about its nominal value, and the thermodynamic-transfer parameter pair (β, υ) is reasonably known [in fact, υ can be on-line estimated, as part of the temperature secondary control design (Gonzalez and Alvarez, 2005)], the implementation of the nonlinear SF controller (5) needs an estimate $\hat{c}$ of the reactor concentration and the reaction rate function $\rho(c,T,p)$. To avoid the need of $\rho(c,T,p)$, let us assume that the reaction rate is in slowly changing regime with respect to the underlying estimation error dynamics, meaning that the time derivative $\dot{r}(t) \approx 0$ of the reactor rate function $\rho(c(t),T(t),p(t)) = r(t)$ is approximately zero (Alvarez-Ramirez, et al., 2002). Combine this assumption with the dynamic heat balance to obtain the estimation model, write the corresponding calorimetric estimator (Alvarez-Ramirez, et al., 2002; Gonzalez and Alvarez, 2005) (6), incorporate the mass balance with $\rho(c,T,p)$ replaced by its estimate $\hat{r}$, and obtain the estimator

$$\dot{\hat{T}} = \beta\hat{r} + \theta(\hat{T}_e - \hat{T}) - \upsilon(\hat{T} - T_j) + 2\zeta_T\omega_T(y - \hat{T})$$
$$\dot{\hat{r}} = (\omega_T^2/\beta)(y - \hat{T}) \tag{6}$$
$$\dot{\hat{c}} = -\hat{r} + \theta(c_e - \hat{c}), \quad \hat{c}(0) = \hat{c}_0 \tag{7}$$

that yields exponentially convergent estimates, with adjustable (or fixed) rate ω_T/ζ_T (or $\sim \theta$) for the reaction rate (or concentration) (Flores, et al., 2005; Gonzalez and Alvarez, 2005)

$$\hat{r} \xrightarrow{\omega_T/\zeta_T} r, \quad \hat{c}(t) \xrightarrow{\sim\theta} c(t)$$

The nonlinear SF controller (5) with the preceding estimator yields the output-feedback (OF) dynamic controller

$$\dot{\hat{c}} = -\hat{r} + \theta(\hat{c}_e - \hat{c}) \tag{8}$$
$$\dot{\hat{T}} = \beta\hat{r} + \theta(\hat{T}_e - \hat{T}) - \upsilon(\hat{T} - T_j) + 2\zeta_T\omega_T(y - \hat{T}) \tag{9}$$
$$\dot{\hat{r}} = (\omega_T^2/\beta)(y - \hat{T}) \tag{10}$$
$$T_j = \hat{T} + [-k_T(\hat{T} - \bar{T}) - \beta\hat{r} - \theta(\hat{T}_e - \hat{T})]/\upsilon \tag{11}$$
$$\theta = [-k_c(\hat{c} - \bar{c}) + \hat{r}]/(\hat{c}_e - \hat{c}) \tag{12}$$

This controller has been employed to track an optimal transition between two open-loop steady-states, in a reactor of class (1) with monotonic reaction rate (Flores, et al., 2005). It must be pointed out that: (i) the implementation of the preceding output-feedback controller does not need the reaction rate function $\rho(c,T,p)$, (ii) the temperature controller (9,10,11) is linear and can be realized as the combination of a linear PI controller with a filter (Gonzalez and Alvarez, 2005), and (iii) the concentration controller is basically a material balance-based ratio control component that sets θ proportionally to $\hat{r}$ (Gonzalez and Alvarez, 2005).

3.3 Redesigned output-feedback controller

The preceding controller has been designed within a local dynamical framework assuming that the closed-loop reactor operates in a sufficiently small neighborhood of the open-loop unstable and partially observable prescribed steady-state. Accordingly, the concentration estimator component (7) has been designed without measurement injection because the temperature measurement does not contains meaningful information. However, from a nonlocal design perspective two considerations must be made: (i) due to typical state and/or exogenous load disturbances, the reactor state may find itself away from a small neighborhood of the steady-state, and (ii) in such case the onset of the complete observability feature offers the possibility of improving the concentration estimator behavior via temperature measurement injection. Thus, the corresponding nonlocal control redesign problem amounts to redesigning the concentration estimation to exploit the far-from equilibrium innovation capability. In principle, two estimator approaches can be employed to perform the joint reaction rate-concentration estimation task: (i) the Luenberguer-like geometric estimator (GE) (Alvarez, 2000), and (ii) the extended Kalman filter (EKF) (Jazwinski, 1970)(Gelb, et al., 1974).

The GE approach is discarded because its observability matrix is singular or equivalently its gain is infinite in the curve Ω (2) (where $\rho_c = 0$) where the nominal steady-state is, and the EKF is disregarded because its observability index equal to two is against the robustness specification of the control design. Instead, a constructive-like hybrid GE-EKF concentration estimation approach will be pursued according to the following rationale: (i) retain the passive-like reaction rate estimation structure (6), and (ii) in a way that is analogous to the design of robust nonlinear controllers via passivation by backstepping using a virtual control to overcome the high relative (say two) obstacle (Krstic, 1995), regard the (quick) reaction rate estimate $\hat{r}$ (10) as a virtual measurement for the concentration dynamics, according to the expressions

$$\dot{\hat{c}} = -\hat{r} + \theta(\hat{c}_e - \hat{c}) \qquad \hat{r} = \rho(\hat{c}, \hat{T}, \hat{p})$$

The corresponding passivated EKF is given by

$$\begin{aligned} \dot{\hat{c}} &= -\hat{r} + \theta(\hat{c}_e - \hat{c}) + g(\hat{c}, \hat{T}, \hat{p}) \left[\hat{r} - \rho(\hat{c}, \hat{T}, \hat{p})\right] \\ \dot{s} &= -2\theta s + \nu - \rho_c^2(\hat{c}, \hat{T}, \hat{p}) s^2, \quad s(0) = s_0 \qquad (13) \\ s &= \sigma / q_r, \quad g(\hat{c}, \hat{T}, \hat{p}) = s\rho_c(\hat{c}, \hat{T}, \hat{p}), \quad \nu = q_c / q_r \end{aligned}$$

where q_c (or q_r) is the model (or measurement) noise intensity, σ is the concentration error covariance, and g is the estimator gain. The variable s and the intensity noise quotient ν have been introduced to have ν as the single tuning parameter. It must be pointed out that the gain g vanishes at the curve Ω ($\rho_c = 0$) and is positive (or negative) in the iso(or anti)tonic branch of the reaction rate, where $\rho_c > (or <) 0$, this is,

$$\begin{aligned} g(c^*, \hat{T}, \hat{p}) = 0, \quad g(c < c^*, \hat{T}, \hat{p}) < 0 \\ g(c > c^*, \hat{T}, \hat{p}) > 0, \quad c^* = \kappa(T, p) \end{aligned}$$

These vanishing-gain switching properties ensure the estimator nonlocal convergence, and imply that, as expected, the estimator injection ceases as the reactor approaches the curve Ω that lacks instantaneous nonlinear and local (linear) observability or, equivalently, the estimator behaves in open-loop regime.

Recall the OF controller (8) replace its open-loop estimator by the passivated EKF (13), and obtain the redesigned OF controller:

$$\begin{aligned} \dot{\hat{T}} &= \beta\hat{r} + \hat{\theta}(\hat{T}_e - \hat{T}) - \upsilon(\hat{T} - \hat{T}_j) + 2\zeta_T\omega_T(y - \hat{T}) \\ \dot{\hat{r}} &= (\omega_T^2/\beta)(y - \hat{T}) \\ \dot{\hat{c}} &= -\hat{r} + \hat{\theta}(\hat{c}_e - \hat{c}) + s\rho_c(\hat{c}, \hat{T}, \hat{p}) \left[\hat{r} - \rho(\hat{c}, \hat{T}, \hat{p})\right] \\ \dot{s} &= -2\hat{\theta}s + \nu - \rho_c^2(\hat{c}, \hat{T}, \hat{p}) s^2 \\ \hat{T}_j &= \hat{T} + [-k_T(\hat{T} - \bar{T}) - \beta\hat{r} - \hat{\theta}(\hat{T}_e - \hat{T})]/\upsilon \\ \hat{\theta} &= [-k_c(\hat{c} - \bar{c}) + \hat{r}]/(\hat{c}_e - \hat{c}) \qquad (14) \end{aligned}$$

4. CLOSED LOOP STABILITY AND TUNING

The application of the EKF output feedback controller (14) to the reactor yields the closed-loop dynamics(k_c and k_T and have been defined in (4), and $A_{T,r}$,q_{ϵ_h},q_σ,q_{ϵ_c},q_T,q_c,λ_c are defined on Appendix A):

$$\begin{aligned} \dot{\epsilon}_h =& A_{T,r}\epsilon_h + \\ & q_{\epsilon_h}\left(c, T, r, c_e, T_e, k_c, k_T; e_T, e_c, \epsilon_c, \tilde{c}_e, \tilde{T}_e\right) \qquad (15) \\ \dot{s} =& -2\theta s + q_\sigma(c, T, \nu, s;\ \epsilon_c) \qquad (16) \\ \dot{\epsilon}_c =& -\lambda_c\tilde{c} + q_{\epsilon_c}(c, T, r, c_e, k_c, \nu; \epsilon_h, \epsilon_c, e_c, \tilde{p}, \tilde{c}_e) \qquad (17) \\ \dot{e}_T =& -k_T e_T + q_T\left(k_c, k_T; \epsilon_h, \epsilon_c, \tilde{p}, \tilde{c}_e, \tilde{T}_e\right) \qquad (18) \\ \dot{e}_c =& -k_c e_c + q_c\left(k_c, k_T; \epsilon_h, \epsilon_c, \tilde{p}, \tilde{c}_e, \tilde{T}_e\right) \qquad (19) \end{aligned}$$

where $\epsilon_h = (\tilde{T}, \tilde{r})$, $\tilde{T} = \hat{T} - T$, $\tilde{r} = \hat{r} - r$, $e_c = c - \bar{c}$, $e_T = T - \bar{T}$, $\epsilon_c = \tilde{c} = \hat{c} - c$.

the perturbation terms vanish as follows:

$$\begin{aligned} q_{\epsilon_h}(c, T, r, c_e, T_e, k_c, k_T; 0, 0, 0, 0, 0) &= 0 \\ q_{\epsilon_c}(c, T, r, c_e, k_c, \nu; 0, 0, 0, 0, 0) &= 0 \\ q_T(k_c, k_T; 0, 0, 0, 0, 0) &= 0 \\ q_c(k_c, k_T; 0, 0, 0, 0, 0) &= 0 \\ q_\sigma(c, T, \nu, s; 0) &= 0 \end{aligned}$$

Observe that: (i) equation (18,19) with $(q_T, q_c) = 0$ is the closed-loop reactor dynamics with the exact SF controller (5), (ii) equation (15) [or (17)] describes the temperature-reaction rate [or concentration] estimation error dynamics, and (iii) the Riccati equation (16) enters only the concentration estimation error dynamics. From the application of standard results in Input-to-State (IS) stability analysis (Isidori, 1995; Sontag, 2000), the next proposition follows:

Proposition 1. (Proof sketch in Appendix B)

The closed-loop reactor is IS stable if the control (k_c, k_T) and estimator (ν, ω_T) gains ($\zeta_T = 1.5$) are chosen so that the following low and high gain conditions are met:

i) $k_c, k_T > 0$, ii)$\nu^-(k_c) < \nu < \nu^+(k_c^{-1})$

iii)$\omega_T^-(k_c, k_T) < \omega_T < \omega_T^+(k_c^{-1}, k_T^{-1})$

where $\nu^-, \nu^+, \omega_T^-, \omega_T^+$ are monotonic functions of their arguments. ■

Condition i) says that feedback is necessary for closed loop reactor stability. Condition ii) says that the estimation gain ν(or ω_T) need to be chosen within interval $[\nu^-, \nu^+]$(or $[\omega_T^-, \omega_T^+]$), with bounds depending on (k_c, k_T). Observe that the lower (or upper) limits ν^- and ω_T^- (or ν^+ and ω_T^+) depend proportionally (inversely proportionally) on the control gains k_c and k_T. In other words, the stability conditions can be met by choosing the control gains (k_c, k_T) sufficiently small. From the preceding closed-loop stability discussion the next tuning guidelines follow:

1. Set the control gains equal to the nominal dilution rate, this is: $k_c \approx k_T \approx \theta$ and choose the temperature and concentration estimation gains about three times faster, this is, $\omega_T \approx 3k_T$, $\nu \approx [3k_c]^{\frac{1}{2}}$.

2. Increase ω_T and ν until the behavior becomes oscillatory, at gain pair $(\omega_T, \nu)^*$. Back off and set$(\omega_T, \nu) \approx (\omega_T, \nu)^* /3$.

3. Increase k_c and k_T until the response behavior becomes oscillatory at $(k_c, k_T)^*$. Back off and set $(k_c, k_T) \approx (k_c, k_T)^*/3$.

4. If necessary, adjust the estimator gains.

5. APPLICATION EXAMPLE

The application example was built by recalling the non-monotonic kinetic function from a previous catalytic reactor estimation study (López, et al., 2002), with a modification to obtain a case where the unstable steady-state coincided with the point that yielded the maximum reaction rate at a prescribed temperature. The non-monotonic reaction function is given by:

$$\rho(c,T,p) = cke^{-\gamma/T}/\left(1+\sigma c\right)^2, \quad c^* = 1/3$$

The operation conditions are listed in Table 1. There are three steady-states, two stable ones S_I(ignition) and S_E(extinction), and one unstable U. The related phase portrait is presented in Fig. B.1. The control input θ(or T_j) is constrained to take values in [0.1,1.2] (or [300,500]). The application of the tuning guidelines yielded the gains: $\zeta_T = 1.5$, $\omega_T = 16$, $k_c = 3$, $k_T = 3$, and $\nu = 3.7$. The reactor was ran from different initial conditions in growing regions about the nominal steady-state $\bar{x}$ finding that: (i) the controller without saturation stabilized the reactor in a rather ample region of initial states (x_0) about $\bar{x}$ ($T_0 \in [416, 456], c_0 \in [0.1, 0.39]$), (ii) with a more sluggish response, the saturated control stabilized the reactor over a rather large region of initial conditions, (iii) in the cold-reactant deficit region the open-loop (OL) and EKF concentration estimator-based controllers exhibited the same behavior, and (iv) in the hot-reactant surplus region the controller with the EKF outperforms its OL concentration-based counterpart. As expected, the controller with the EKF concentration observer has the (non-local) capability of improving its behavior when the reactor finds itself in the dangerous high temperature region. This situation is illustrated in fig B.2, with initial condition $T_0 = \bar{T} + 6$ and $c_0 = \bar{c} - 0.063$. As it can be seen, both controllers yield the same temperature response, the controller with the OL (or EKF) composition estimator causes the reactor concentration to reach its set point in a 98% setting time in 4 (or 1.25) time units. In other words, in this region the passivated EKF yields a concentration response that is about three times faster than the one of the passive OL (i.e. asymptotic) estimator.

Table 1. Steady states and operation conditions

$k = e^{25}, \gamma = 10e4, \sigma = 3, \theta = 0.989$ $\upsilon = c_e = 1, T_e = T_j = 370, \beta = 200$			
steady states	S_E	U	S_I
concentration [mol/L]	0.991	0.333	0.033
temperature [K]	370.88	436.02	465.25
local condition	stable	unstable	stable

6. CONCLUSIONS

The problem of controlling a continuous reactor with non-monotonic reaction rate, about a (possibly open-loop unstable) steady state with maximum rate and lack of local observability was addressed within a nonlocal constructive design framework. The resulting output-feedback controller was made of passive components: (i) a calorimetric PI temperature controller combined with a linear filter, (ii) a feedforward-like ratio concentration controller driven by the reaction rate estimate, or equivalently, by the integral action of the temperature controller. The unmeasured concentration was regulated via a material balance-based inferential scheme. The lack of local observability and the presence of away-from-equilibrium concentration observability were handled by a passivated concentration EKF driven by the quickly convergent reaction rate estimate acting as a virtual measurement. The closed-loop behavior of a representative case through simulations corroborated the nonlocal robust functioning of the proposed controller.

Appendix A. NONLINEAR MAPS

$$A_{T,r} = \begin{bmatrix} -k_T - 2\zeta_T\omega_T & \beta \\ 0 & -\dfrac{\omega_T^2}{\beta} \end{bmatrix}, \quad \lambda_c = k_c\left(1+\frac{1}{c_e-c}\right) + \hat{g}\,\mathrm{sec}_{\tilde{c}}^{\rho}$$

$$\mathrm{sec}_c^{\rho} = \frac{\rho\left(c+\tilde{c},T,p\right)-\rho\left(c,T,p\right)}{\tilde{c}}, \quad q_{\epsilon_h} = [q_T, q_r]^T$$

$$q_T = (T-T_e)\left(\hat{\theta}-\theta\right) + \gamma\left(\hat{T}_j - T_j\right)$$

$$q_r = \rho_c(c,T,p)k_c(e_c+\tilde{c}) - \rho_c(c,T,p)q_c(c,T,r,c_e;\tilde{c},\tilde{T},\tilde{r},\tilde{c}_e)$$

$$q_\sigma = \nu + \rho_c(c-\hat{c},T,\hat{p}), \quad q_{e_c} = -\tilde{r} + \left(\hat{\theta}-\theta\right)(\tilde{c}_e - \tilde{c})$$

$$q_{\epsilon_c} = -g(\hat{c},\hat{T},\nu)\left[\rho(\hat{c},\hat{T},p+\tilde{p}) - \rho(\hat{c},T,p)\right] - \tilde{r} - (\tilde{c}_e)\left(\hat{\theta}-\theta\right)$$

$$q_{e_T} = \beta\tilde{r} + \left(\hat{\theta}-\theta\right)\left(\tilde{T}_e - \tilde{T}\right) - \delta\left(\tilde{T}+\tilde{T}_j\right)$$

Appendix B. SKETCH OF THE PROOF OF PROPOSITION 1.

The proof of Proposition 1 follows from the application of two well known results:

Theorem 1. (Sontag, 2000) The system

$$\dot{x} = f(x,u),\ f(0,0) = 0 \qquad \text{(B.1)}$$

is IS stable if: (a) the zero input system $x = f(x,0)$ is zero-stable, and (b) the system with input has an asymptotic gain λ_u^x. ■

Theorem 2. (Small gain) (Isidori, 1995) Consider two IS stable systems (with convergence parameters λ_x and λ_y) $\dot{x} = f(x, y, u)$ λ_x $\dot{y} = g(x, y, u)$ λ_y The interconnection of the systems is IS stable if:

$$(a_x L_y^f /)(a_y L_x^g /) < 1 \quad .\blacksquare$$

where L_y^f denotes the Lipschitz constant of f with respect to y. Further technical details on the application of the theorems can be seen in (Gonzalez and Alvarez, 2005), here we circumscribe ourselves to sketch the proposition proof: (i) Apply Theorem 1 to ensure the stability for each subsystem of the error dynamics (15-17). (ii) Successively apply Theorem 2 to draw the stability condition for the closed-loop reactor dynamics (15-19).■

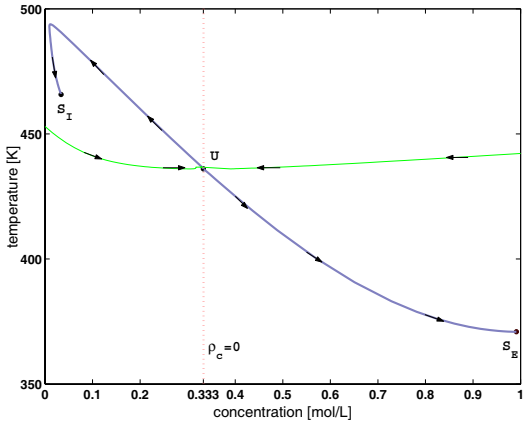

Fig. B.1. Open-loop reactor behavior

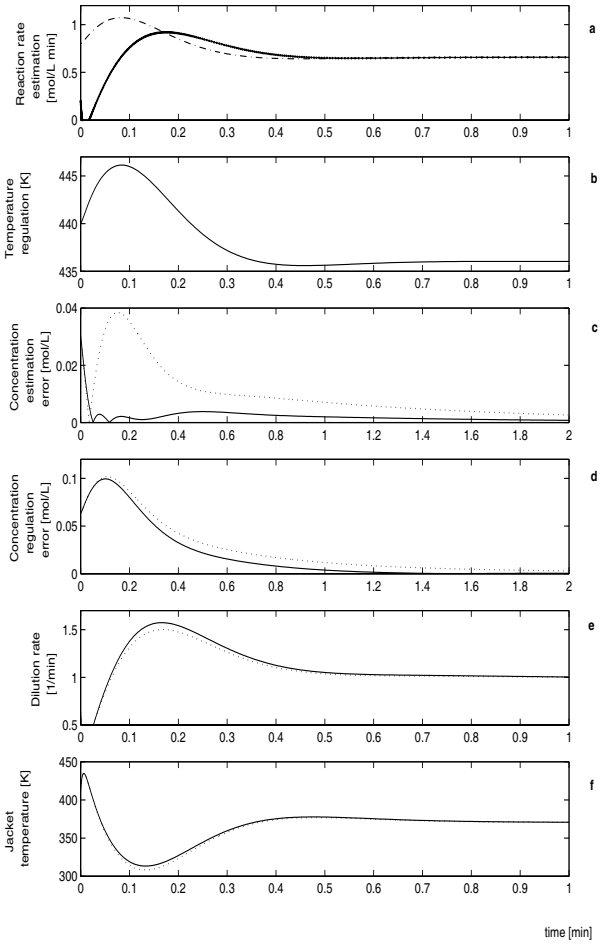

Fig. B.2. (a) Actual (-·) and reaction rate estimators with passive OL (–) and passive EKF (··) concentration estimator. (b) Temperature regulation. (c-f) Closed loop with OL (··) and EKF (–) passive concentration observers

REFERENCES

Alvarez, J., Nonlinear state estimation with robust convergence, *J. of Process Control*, v 10, n 1, p 59-71, 2000.

Alvarez-Ramirez, J., Alvarez, J., Morales, A., An adaptive cascade control for a class of chemical reactors, *I. J. of Adaptive Control and Signal Processing.* 16:681-701, 2002.

Elnashaie, S., Abashar, M., The implication of non-monotonic kinetics on the design of catalytic reactors, *Ch. Eng. Sc.* Vol. 45, No. 9, pp. 2964-2967, 1990.

Flores-Tlacuahuac, A., Alvarez, J., Saldivar-Guerra E., Oaxaca, G., Optimal transition and robust control design for exothermic continuous reactors, *AIChEJ.* Vol. 51, Is. 3, 2005.

Gelb, A., Kasper, J., Nash, R., Price, C., Sutherland, A., *Applied Optimal Estimation.* MIT press cambridge, MA, 1974.

González, P., Alvarez, J., Combined PI-inventory control of solution homopolymerization reactors, *Ind. & Eng. Chem. Res. J.* 2005.

Hermann, R., Krener, A.J., Nonlinear controllability and observability, *Trans. on Aut. Control.* IEEE, p 728-740, 1977.

Isidori, A., *Nonlinear Control Systems.*, Spinger, New York, 1995.

Jazwinski, A.H., *Stochastic Processes and Filtering Theory.* Academic Press, New York, 1970.

Krstic, M., Kanellakopoulos, I., Kokotovic, P., *Nonlinear and Adaptive Control Design.*Wiley, New York, 1995.

Lapidus, L.,Amundson, N. Editors *Chemical Reactor Theory.* Prentice Hall, New jersey, 1977.

Lopez, T., Tronci, S., Baratti, R., Alvarez, J., State estimation in a Catalytic Reactor via a Constructive Approach, *15th Triennial World Congress*, 2002.

Smets, I., Bastin, G., Van Impe, J., Feedback Stabilization of Fed-Batch Bioreactors: Non-Monotonic Growth Kinetics, *Biothecnol. Prog.* 18,p. 1116-1125, 2002.

Sontag, E.D., The ISS Phylosophy as a unifying Framework for Stability-like Behavior, in Nonlinear Control in the year 2000, Vol 2., *Lecture Notes in Control and Information Sciences.* Berlin, 2000.

Zeitz, M., The extended Luenberger observer for nonlinear systems, *Systems & Control Letters.* 9 pp. 149-156, 1987.