OUTPUT-FEEDBACK DISSIPATIVE CONTROL OF EXOTHERMIC CONTINUOUS REACTORS

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Abstract: The problem of controlling a (possibly open-loop unstable) continuous exothermic reactor with temperature measurements and manipulation of reactant feed and heat exchange rates is addressed within a passivity-dissipativity framework. The combination of a nonlinear passive state-feedback (SF) controller with a dissipative observer yields the dissipative output-feedback (OF) controller closed-loop stability conditions with: (i) the identification of the underlying gain-behavior interplay, and (ii) simple tuning guidelines. The approach is tested through numerical simulations, with a representative worst-case example: an exothermic reactor with Langmuir-Hinshelwood nonmonotonic kinetics, which must be regulated about an open-loop unstable steady-state which is not observable.

Keywords: Chemical Reactor Models, Output-Feedback Control, Dissipativity, Observability.

1. INTRODUCTION

Continuous exothermic chemical reactors are complex nonlinear dynamical systems with nonlinear behavior, asymmetric MIMO coupling, parametric sensitivity, multiplicity, hysteresis, bifurcation, and limit cycling. Most of the industrial reactors are controlled by combining conventional (ratio, and cascade) feedforward and (P, PI and PID) feedback linear control component with supervisory or advisory material-energy balance and optimizing controllers (Shinskey [1988], Gonzalez and Alvarez [2005]). The process design or redesign to meet tighter safety, productivity, quality and environmental requirements motivates the development of more capable and systematic reactor control designs. Advanced nonlinear control studies have been performed in the chemical process systems engineering field, the related state of the art can be seen elsewhere, and here it suffices to mention that: (i) with a few exceptions (Alvarez et al. [1991], Viel and Jadot [1997], Antonelli and Astolfi [2003]) most of the studies lack rigorous stability and performance assessments, and (ii) only the optimality-based MPC (which stems from industrial control developments) has reached the stage of acceptance for plant scale testing or implementation (Eaton and Rawlings [1990]). Recently, in the context of polymer reactor (Gonzalez and Alvarez [2005], Diaz-Salgado et al. [2007]) and distillation column output-feedback control studies (Castellanos-Sahagun and Alvarez [2006]) with constructive nonlinear control, connections between PI, inventory and MP control designs have been identified, and the closed-loop stability assessment and tuning aspects have been handled either with conceptual arguments or with the small gain theorem. The dissipativity notion offers a unifying framework to handle design-oriented tools in constructive control (Sepulchre et al. [1997]) according to fundamental connections between optimality, passivity, robustness and dissipativity, with emphasis on interlaced observer-control designs and rigorous stability assessments. The dissipativity ideas (i) were originally developed in the context of state-feedback (SF) control problems (Willems [1972]), (ii) have been extended to design of nonlinear observers (Moreno [2005]), and observer-control separation (Moreno [2006]), and (iii) enable the tackling of the difficult problem of estimating and controlling reactors with non-monotonic kinetics, and lack of observability at maximum reaction rate (Schaum et al. [2008]).

The preceding considerations motivate the present reactor output-feedback (OF) control study, where the problem of controlling a continuous exothermic (possibly open-loop unstable) reactor with either monotonic or non-monotonic kinetics, temperature measurements, and manipulation of reactant and heat exchange rates is addresed within a combined passivity-dissipativity approach, including (i) the derivation of rigorous closed-loop stability conditions coupled with easy-to-apply tuning guidelines, and (ii) the identification of the underlying interplay between regulation speed, robustness, and observer-control gains. The proposed approach is tested, through numerical simulations, with an exothermic reactor with nonmonotonic kinetics, open-loop instability, and lack of observability.

In our previous study (Schaum et al. [2008]) the reactor problem was adressed by *ad hoc* combining a passive controller with a dissipative observer, and drawing closed-loop stability conditions with the small gain theorem. However, the passivity (controller) and dissipativity (observer) approaches were methodologically disconnected, and the stability characterization was not reflected in a practical tuning. In the present work: (i) the controller-observer design and the closed-loop stability assessment are performed with a united framework, and (ii) a simple tuning scheme that is clearly related with closed-loop functioning features is obtained .

2. CONTROL PROBLEM

Consider a continuous chemical reactor where a reactant is converted into product via an exothermic reaction, heat being removed through a diathermal wall with a cooling jacket. Assuming the volume (V) and the jacket temperature (T_c) are controlled with fast (conventional, linear decentralized) feedback loops which manipulate the exit and coolant flowrates (Shinskey [1988]) the *reactor model* is given by the dynamic mass-energy balance:

$$\begin{aligned} \dot{c} &= -r(c,T,\pi) + \theta(c_e - c), & c(0) &= c_0 \\ \dot{T} &= \beta r(c,T,\pi) + \theta(T_e - T) - \eta(T - T_c), & T(0) &= T_0 \end{aligned} \quad (1)$$

where ($\bar{(\cdot)}$ is the steady-state (SS) value of $(\cdot)$)

$$\begin{aligned} & c = C/C^0, \quad \theta = q/V, \quad \beta = (-\Delta H)C^0/(V\rho_m c_p) \\ & \eta = (UA_U)/(V\rho c_p), \quad p = (p_a', \pi')', \quad p_a = (c_e, \beta, \eta)' \\ & r(\bar{c},\bar{T}) + \bar{\theta}(\bar{c}_e - \bar{c}) = 0, \\ & \beta r(\bar{c},\bar{T},\pi) + \bar{\theta}(\bar{T}_e - \bar{T}) - \eta(\bar{T} - \bar{T}_c) = 0 \end{aligned}$$

The reactant dimensionless concentration c, and the reactor temperature T are the states, the dilution rate q and the jacket temperature T_c are *control inputs*, r is the nonlinear reaction rate function, π is its parameter vector, θ is the inverse residence time, η is the heat transfer coefficient-to-capacity quotient, β is the adiabatic temperature rise, the feed concentration c_e and temperature T_e are the *exogenous inputs*, C (or C^0) is the reactant (or pure reactant) concentration, q is the feed flowrate, $-\Delta H$ is the heat of reaction, ρ_m (or c_p) is the reacting mixture density (or specific heat capacity), U (or A_U) is the heat transfer coefficient (or area), and p is the model parameter. The temperatures (T and T_c) are measured, and the concentrations (c_e and c) are not. In compact vector notation the *reactor model* (1) is given by

$$\dot{x} = f\left[x, d(t), u, p\right], \quad x(0) = x_0, \quad y = Cx, \quad z = x \quad (2)$$

$$\begin{aligned} & x = [c,T]' \in X = [0,1] \times (T^-, T^+) \subset \mathbb{R}^2, \quad p = (p_a', \pi')' \\ & f[\bar{x},\bar{d},\bar{u},p] = 0, \quad d = [c_e, T_e]', \quad T_e = y_e - \tilde{y}_e, \ C = [0,1], \\ & u = (\theta, T_c), \ T^- = \min(T_e, T_c), \ T^+ = \max(T_e, T_c) + \beta \end{aligned}$$

x is the state, u (or d) is the control (or exogenous, possibly time-varying) input, and y (or z) is the measured (or regulated) output. X is an invariant set, meaning that all state motions born in X stay in X (Alvarez et al. [1991]). Since the reactor model (1) contains constant ($\tilde{p}$) and time-varying reactor (or feed) temperature measurement $\tilde{y}$ (or $\tilde{y}_e$), and dilution rate ($\tilde{\theta}$ (or coolant temperature ($\tilde{T}_c$)) actuator bounded errors, the *actual reactor system dynamics* are given by

$$\begin{aligned} & \dot{x} = f[x, d + \tilde{d}(t), u + \tilde{u}(t), p + \tilde{p}], \\ & x(0) = x_0, \quad y = Cx + \tilde{y}(t), \quad z = x \end{aligned} \quad (3)$$

$$\begin{aligned} & \tilde{p} = (\tilde{p}_a, \tilde{\pi}), \ \tilde{d}(t) = [\tilde{c}_e(t), \tilde{y}_e(t)]', \ \tilde{u}(t) = [\tilde{\theta}(t), \tilde{T}_c(t)]', \\ & \tilde{y}(t) = y - T|\tilde{p}| \le \delta_p, \quad ||\tilde{d}(t)|| \le \delta_d, \quad ||\tilde{u}(t)|| \le \delta_u, \\ & ||\tilde{y}(t)|| \le \delta_y, \quad ||(.)(t)|| = \sup_{t\in[0,\infty)} |(.)(t)|, \end{aligned}$$

where δ_p, δ_d, δ_u and δ_y are the error sizes, and $|(\cdot)|$ is the Euclidian norm of the vector $(\cdot)$. Our *control problem* consists in designing, on the basis of the reactor model (1) (with parameter approximation p) and flow and temperature measurement, an observer-based dynamical *output-feedback (OF) controller* to regulate the concentration-temperature pair z, about a (possibly opn-loop unstable and unobservable) SS by manipulating the dilution rate-cooling temperature pair u.

3. OUTPUT-FEEDBACK (OF) CONTROLLER

The reactor dynamics represent mass and energy accumulation due to advective, reaction and heat exchange input/output mechanisms. From the abstract energy perspective associated with the dissipativity control (Willems [1972], Sepulchre et al. [1997]) and estimation (Moreno [2005]) framework, our OF control problem amounts to designing the observer-control pair in such a way that the dissipation rate is negative, and robust, and implies nonwasteful control action.

In deviation form referred to the SS regime, the reactor system (1) is written as follows

$$\begin{aligned} & \dot{e} = f_e[e, \tilde{u}_e(t)], \ e(0) = e_0, \ e = x - \bar{x}, \\ & \tilde{u}_e = (\tilde{p}', \tilde{d}', \tilde{u}')', \ f_e(0,0) = 0. \end{aligned} \quad (4)$$

According to the definition of *nonlocal input-to-state stability (ISS)* (Freeman and Kokotovic [1996]), the SS $e = 0$ is said to be *practically uniformly* (P) *stable* if an admissible disturbance size (δ_u) produces an admissible state deviation size (ε_x): given (δ_u, ε_x) there is a KL-class (increasing-decreasing) function β and a K-class (increasing) γ so that the state responses of system (4) are bounded as follows

$$\begin{aligned} & |e_0| \le \delta_0, |\tilde{u}_e(t)| \le \delta_u, \quad (5) \\ & \Rightarrow |e(t)| \le \tau(|e_0|, t) + \alpha(||\tilde{u}_e(t)||) \le \tau(\delta_0, 0) + \alpha(\delta_u) = \varepsilon_x \end{aligned}$$

where τ (or α) bounds the transient (or asymptotic) response. The (necessary and sufficient) Lyapunov characterization of the ISS property is given by

$$\alpha_1(|e|) \le V(e) \le \alpha_2(|e|), \quad \dot{V} = -\alpha_3(|e|) + \alpha_4(|\tilde{u}_e|) \quad (6)$$

where V is a positive definite radially unbounded function and $\alpha_1, \cdots, \alpha_4$ are K-class functions.

3.1 Passive state-feedback (SF) controller

The notion of *passivity* plays a key role in the design of robust nonlinear SF controllers (Khalil [2002]), with: (i) fundamental connections between optimality, robustness and passivity, and (ii) means to analytically construct optimal controllers via inverse optimality. An optimal SF controller is passive and underlien by a minimum phase (MP) system (with relative degree less or equal than one). A nonlinear system is passive if it is *dissipative* (Willems [1972]) with storage function-supply rate pair and MP.

The reactor (1) is feedback-passive (after input coordinate change) with respect to the input-output pair (u, z) and the storage function $V = e^T e$ if and only if the reactor relative degree equal to one condition is met, i.e. (Schaum et al. [2008]):

$$\text{rd}(u,z) = (1,1), \ z = x \ \Leftrightarrow c_e \ne c \ , \ \eta \ne 0 \quad (7)$$

Thus, the state-input coordinate change $e = x - \bar{x}, v = f(x,d,u)$ takes the reactor into the passive normal form (8)

$$\dot{e} = v, e(0) = e_0, \psi = e; V = e^T e, \dot{V} = 2\psi^T v, \quad (8)$$

with storage function V and input-output pair (v, ψ). The SF controller (9) yields the closed-loop (decoupled, stable, and dissipative) dynamics (10),

$$v{=}f(e, d, u){=}{-}Ke, K{=}\text{diag}(k_c, k_T) \Rightarrow u{=}\mu(x, d, u) \quad (9)$$

$$\dot{e}{=}{-}Ke, e(0){=}e_0, \psi{=}e; V{=}\ e^T e, \dot{V}{=}{-}2eTKe < 0. \quad (10)$$

In original coordinates, *the nonlinear passive SF controller* (9) is given by:

$$\begin{aligned} &\theta = [r(c,T) - k_c(c - \bar{c})]/(c_e - c), \\ &T_c = T - [\beta r(c,T) + \theta(T_e - T) + k_T(T - \bar{T})]/\eta \end{aligned} \quad (11)$$

This controller with state, parameter, and measurement-actuator errors $(\epsilon, \tilde{d}, \tilde{p})$, yields the closed-loop dynamics (13) with dissipation (14)

$$u = \mu(x + \epsilon, d + \tilde{d}, p + \tilde{p}) := [\mu_\theta, \mu_{T_c}]^T \quad (12)$$

$$\dot{e} = -Ke + \tilde{f}\Big[e; \epsilon, \tilde{d}(t), \tilde{p}\Big], e(0){=}e_0, K{=}\ \text{diag}(k_c, k_T) \quad (13)$$

$$\dot{V} \leq -2\min\{k_c, k_T\}V + e'\tilde{f}\left[e; \epsilon, \tilde{d}(t), \tilde{p}\right] \quad (14)$$

$$\tilde{f}\left(e; \epsilon, \tilde{d}, \tilde{p}\right) = f\left[\bar{x} + e, \bar{d} + \tilde{d}, \mu\left(x + \epsilon, \bar{d} + \tilde{d}, p + \tilde{p}\right), p\right]$$

$$e = (e_c, e_T)' = x - \bar{x}, \quad \tilde{f}(e; 0, 0, 0) = 0.$$

Since the reactor has trivially stable nominal zero-dynamics $e = 0$, the errorless closed-loop is asymptotically stable. From the Lipschitz continuity of (f, μ) the system P-stability follows (Khalil [2002]), with a suitable tradeoff between the initial state (δ_0), parameter (δ_p), input (δ_d and $\delta_{\tilde{x}}$) and state excursion (ε_x) sizes, depending on the choice of the control gain pair (k_c, k_T). The P-stable closed-loop reactor dynamics (13) represents: (i) the behavior attainable with any robust controller, and (ii) the recovery target for the OF control design. The related solvability conditions (7) are generically met by the reactor class (1) because: (i) $c < c_e$, and (ii) $\eta > 0$.

3.2 Dissipative observer

The nonlinear global detectability property of any reactor motion (Schaum et al. [2008]) suggests the consideration of a dissipative observer, because (i) its functioning does not require complete observability (Moreno [2005]), and (ii) the structure-oriented approach offers a means to perform the control-estimator design (Section 4). The reactor dissipative observer is given by (Schaum et al. [2008])

$$\begin{aligned} &\dot{\hat{c}} ={-}r[\hat{c} - \kappa_r(\hat{T} - y), y, \pi] + \theta(c_e - \hat{c}) - \kappa_c(\hat{T} - y), \\ &\dot{\hat{T}} = \beta r[\hat{c} - \kappa_r(\hat{T} - y), y, \pi] + \theta(T_e - \hat{T}) - \\ &\qquad\qquad -\eta(\hat{T} - T_c) - \kappa_T(\hat{T} - y), \\ &\hat{c}(0) = \hat{c}_0, \quad \hat{T}(0) = \hat{T}_0, \end{aligned} \quad (15)$$

where κ_c (or κ_T) is the usual concentration (or temperature) gain, and κ_r is the gain of an injection in the concentration argument of the reaction rate. The estimation error dynamics are given by the two-subsystem interconnection in Lur'e- Popov form (Khalil [2002], Willems [1972], Schaum et al. [2008])

$$\begin{bmatrix} \dot{\varepsilon}_c(T) \\ \dot{\varepsilon}_T(t) \end{bmatrix} = \begin{bmatrix} -\theta(t) & -\kappa_c \\ 0 & -\lambda_T \end{bmatrix} \begin{bmatrix} \varepsilon_c(T) \\ \varepsilon_T(t) \end{bmatrix} + \begin{bmatrix} 1 \\ -\beta \end{bmatrix} \nu \quad (16)$$

$$\psi = \zeta \triangleq \epsilon_c - \kappa_r\epsilon_T,, \quad \lambda_T \triangleq \theta(t) + \eta + \kappa_T$$

$$\nu = -\rho\,(c, y; \zeta)\,, \quad (17)$$

with (i) a linear-dynamic advective subsystem (16) with input ν and output ζ, and (ii) a nonlinear-static kinetic subsystem (17) with the reaction rate error. Since the rate r is continuously differentiable, there is a continuous secant function φ so that the estimated minus the actual rate is conically bounded (18) with the nonlinearity ρ is encompassed in the conic sector (19)

$$\rho(c, T; \zeta) \triangleq r\,(c + \zeta, T) - r(c, T) = \varphi\,(c, T; \zeta)\,\zeta, \quad (18)$$

$$\zeta \triangleq \epsilon_c - \kappa_r\epsilon_T, \quad -k_1\,(T) \leq \varphi\,(c, T; \zeta) \leq k_2\,(T)$$

$$-\,k_1\,(T) = \min_{0\leq c\leq 1} r_c(c, T, \pi)\ , k_2\,(T) = \max_{0\leq c\leq 1} r_c(c, T, \pi),$$

$$(k_2\zeta - \rho(c, T; \zeta))\,(\rho(c, T; \zeta) + k_1\zeta) \geq 0 \quad (19)$$

(Khalil [2002]). Consequently, the static system (17) is $[-1, 1/2(k_2 - k_1), -k_1k_2]$-dissipative Moreno [2005], and its dissipation is characterized by the reaction rate slopes: the slope k_1 is positive (or negative) if the reaction rate is monotonic (or non-monotonic). The observer is designed in such a way that: (i) the open-loop estimation error dynamics consist of the feedback interconnection of two adequatly dissipative (passive) subsystems, and (ii) the estimator and control dissipativity properties are structurally compatible. The observer gains $\kappa_c, \kappa_T, \kappa_r$ are chosen so that the system interconnection (16) - (17) is dissipative with respect to the estimation storage function

$$\hat{V} = \frac{1}{2}\epsilon^T\epsilon. \quad (20)$$

The gain pair (κ_c, κ_T) shapes the dissipation of the linear dynamical subsystem, and the gain κ_r determines the interconnection form by setting the output of the linear system. Convergence conditions for the dissipative open-loop observer (15) are given in (Schaum et al. [2008]).

3.3 OF controller

The combination of the SF (9) passive nonlinear controller with the dissipative observer (15) yields the *dynamic OF controller*

$$\begin{aligned} &\dot{\hat{c}} ={-}r[\hat{c} - \kappa_r(\hat{T} - y), y, \pi_r] + \theta(c_e - \hat{c}) - \kappa_c(\hat{T} - y)\ , \\ &\dot{\hat{T}} = \beta r[\hat{c} - \kappa_r(\hat{T} - y), y, \pi_r] + \theta(T_e - \hat{T}) - \\ &\qquad\qquad -\eta(\hat{T} - T_c) - \kappa_T(\hat{T} - y), \\ &\theta = [r(\hat{c}, T) - k_c(\hat{c} - \bar{c})]/(c_e - \hat{c}), \\ &T_c = \hat{T} - [\beta r(\hat{c}, T) + \theta(T_e + \hat{T}) + k_T(\hat{T} - \bar{T})]/\eta \end{aligned} \quad (21)$$

with five adjustable gains: k_c and k_T for the passive-dissipative controller, and κ_c, κ_T and κ_r for the observer.

4. CLOSED-LOOP STABILITY AND TUNING

In this section, the closed-loop dynamics are characterized, yielding: (i) stability conditions, (ii) tuning guidelines, and (iii) a functioning assessment. The main difficulty resides in an inherent limitation: the unmeasured output concentration (c) must be regulated about a steady-state wich is open-loop unstable and not locally observable.

The application of the OF controller (21) to the actual reactor (3) yields the *closed loop dynamics*

$$\begin{aligned} &\dot{e} = -Ke + \psi(e)\epsilon + \phi\left(e, \epsilon; \tilde{d}(t), \tilde{p}\right), \\ &\dot{\epsilon} = M(t)\epsilon + \tilde{g}\left(e, \epsilon; \tilde{d}(t), \tilde{p}\right), \end{aligned} \quad (22)$$

$$M(t) = \begin{bmatrix} -\theta(t) - \varphi(t) & -\kappa_c \\ \beta\varphi(t) & -\lambda_T \end{bmatrix},\ \phi\,(e; 0) = 0$$

where e (or ϵ) is the regulation (or estimation) error, ϕ results from the replacement of ϵ_T by $\tilde{y}$ in the reaction rate term of the error function $\tilde{f}$ (13) associated with the Lyapunov closed-loop stability characterization with SF control. From the continuity of ϕ, $\tilde{f}$, $\tilde{g}$ and the compactness of their domains their Lipschitz continuity and boundedness follow.

Given that the separation principle holds for linear but not for nonlinear systems, the nominal closed-loop stability (i.e. system (22) with $(\tilde{g}, \phi) = (0, 0)$) can be established as follows: since the regulation error dynamics are individually P-stable and the estimation error dynamics are individually convergent, the reactor(1)-OF controller(21) interconnection is uniformly asymptotically stable (Angeli et al. [2004], Moreno [2006]). Motivated by the need of a more constructive stability criterion in the sense of practical applicability for gain tuning and behavior assessment purposes, in the next propositionclosed-loop stability conditions are given in terms of the five-gain set $(k_c, k_T, \kappa_c, \kappa_T, \kappa_r)$ of the proposed OF controller (21).

Proposition 4.1. (Sketch of proof in Appendix A) The closed-loop reactor (1) with the proposed passive-dissipative OF controller (22) is P-stable if the controller five-gain set $(k_c, k_T, \kappa_c, \kappa_T, \kappa_r)$ and the regulation-estimation error set meet the conditions

$$(i)\ \theta = \mu_\theta(k_c) > -k_1, \qquad (ii)\ k_c > \iota_c(k_c)$$
$$(iii)\ k_T > \iota_T(k_c, \kappa_c, \kappa_r), \quad (iv)\ \kappa_T > \iota_\tau(k_c, k_T, \kappa_T, \kappa_c, \kappa_r),$$

with μ_θ givn in (12) and $\iota_c, \iota_T, \iota_\tau$ in Appendix A.

As it can be seen in Appendix A, the combined passivity-dissipativity approach enables the derivation of the above stability conditions in a rather straighforward way, by using the passive control (V) (13) and dissipative observer $(\hat{V})$ (20) storage functions and applying Lyapunovs direct method. In the absence of modeling error the closed-loop stability becomes asymptotic. Condition (i) is a closed-loop detectability requirement, Condition (ii) ensures the stability of the regulation-estimation concentration dynamics and imposes lower and upper limits ($k_c^- \approx 1, k_c^+ \approx 3$) on the composition control gain k_c (Gonzalez and Alvarez [2005]), and Conditions (iii) and (iv) ensure the stability of the regulation-estimation temperature dynamics and of the entire interconnection. Thus, for $\kappa_r \approx 1/\beta, k_c \approx 3\bar{\theta}$, the preceding inequality conditions can be met by choosing: (i) k_T sufficiently large to dominate $\iota_T(k_c, \kappa_c, \kappa_r)$, and (ii) κ_T sufficiently large to dominate $\iota_\tau(k_c, k_T, \kappa_c, \kappa_r)$.

From the preceding P-stability conditions the conventional-like tuning guidelines follow: (i) set the gains conservatively at $(k_c, k_T) \approx (1, 3), \kappa_r \approx 1\beta, \kappa_c \approx k_c, \kappa_T \approx 10\kappa_c$, (ii) increase the T-estimation gain κ_T until oscillatory response is obtained at κ_T^+, back off and set $\kappa_T = \kappa_T^+/2$-to-3, (iii) in the same way set $k_T = k_T^+/2$-to-3, (iv) carefully increase k_c (sufficiently below $k_c^+ \approx 4\bar{\theta}$) until there is no improvement, and adjust κ_r. If necessary, repeat steps (ii) to (iv).

The solvability of the robust OF reactor control problem is a consequence of: (i) the solvabilities of the OF control (7) and dissipative closed-loop observer (condition (i) in Proposition 4.1) problems, and (ii) the adequate choice of gains according to Proposition 4.1.

5. APPLICATION EXAMPLE

To subject the proposed OF controller to a severe test, let us consider an extreme case of an industrial situation: the operation of the continuous reactor (3) with the Langmuir-Hinshelwood (LH) kinetics model

$$r(c, T, \pi) = \frac{cke^{-(\frac{\gamma}{T})}}{(1 + \sigma c)^2}, \quad r_c = (c^*, T, \pi) = 0, c^* = 1/\sigma$$

adapted from a previous (partial open-loop or asymptotic and full measurement injection) estimation study with EKF and experimental data for the catalyzed carbon monoxide oxidation reaction (Baratti et al. [1993]). With the nominal parameters and inputs

$$\bar{d}' = (\bar{c}_e, \bar{T}_e) = (1, 1), \bar{u}' = (\bar{\theta}, \bar{T}_c) = (1, 370), p = (p_a', \pi')',$$
$$p_a = (\bar{c}_e, \bar{T}_e, \eta)' = (1, 370, 1), \pi' = (k, \gamma, \sigma) = (e^{25}, 10000, 3)$$

the reactor has three steady-states (Diaz-Salgado et al. [2007]: two stable (extinction and ignition), and one unstable at maximum concentration rate $r^* = 0.6614$ with $c^* = 1/3$. The application of the tuning guidelines associated with Proposition 4.1 yielded: $\kappa_c = 0.62$, $\kappa_T = 30$, $\kappa_r = \frac{1}{50}$, $k_c = 2$, $k_T = 3.$, and the initial reactor and estimator conditions were set at $x_0 = [430, 0.28]'$, $\hat{x}_0 = [425, 0.35]'$, about the unstable steady-state with maximum rate. The relative degree (7) and global detectability (Schaum et al. [2008]) conditions are well met, because: $c_e - \bar{c} = 2/3 > 0, \eta = 1 > 0, \bar{\theta} = 1, 1/3 = \theta^- \leq \theta \leq \theta^+ = 3/2$. In the spirit of the nonlocal P-stability framework, the closed-loop reactor with nominal SF, nominal and perturbed OF will be subjected to initial state, and persistent parameter and exogenous input disturbances.

5.1 Nominal behavior with SF control

The closed-loop reactor behavior with exact model-based nonlinear passive SF controller (9) is shown in Figure 1. As expected, the concentration (or temperature) response is about one half (or quarter) settling residence time ($4/\theta = 4$), with smooth-coordinated dilution rate-coolant temperature control action, safely away from saturation. This agrees with the optimality-based non-wasteful feature of passive SF controllers (Sepulchre et al. [1997]).

5.2 Nominal behavior with OF control

Initially, the reactor was in the above stated deviated initial state, and subjected to known constant feed concentration $c_e = 1$ and temperature $T_e = 370K$. The behavior with exact model-based OF control (21) is shown in Figure 2: (i) the state responses are quite similar to the ones of the nonlinear SF controller (Figure 1), in spite of a sluggish concentration estimate response (about 3/4th of the natural settling time), and (ii) as expected from the FF component of the OF controller, the control inputs practically annihilate the effect of the known oscillatory input, and (iii) the control actions are smooth and efficient, reasonably away from saturation. Thus, the nominal OF controller recovers rather well the behavior of its exact model-based nonlinear SF counterpart. This test verifies

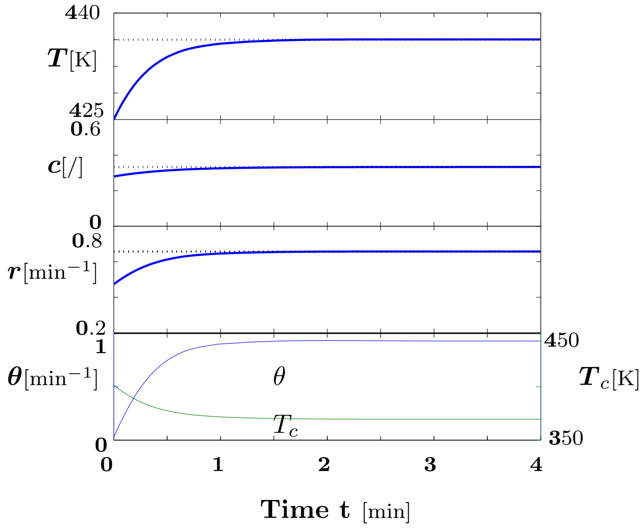

Fig. 1. Closed-loop nominal behavior with nonlinear SF controller: input and response (—) , estimate (– –), and set point (· · ·).

the closed-loop P-stability property with OF dynamic control, with asymptotic convergence to the prescribed SS.

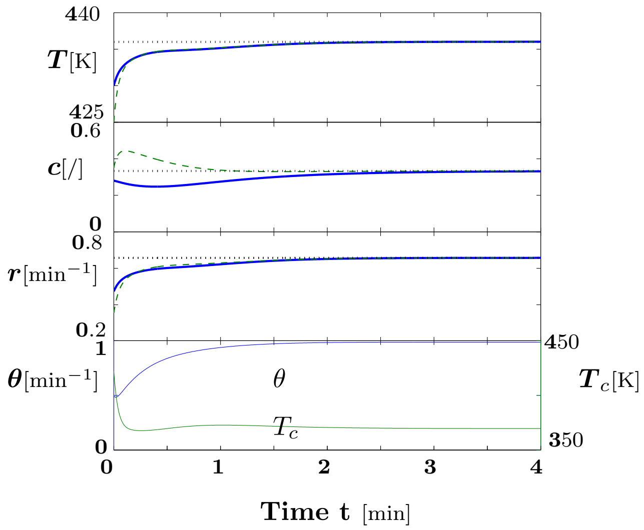

Fig. 2. Closed-loop nominal behavior with nonlinear OF controller: input and response (—) , estimate (– –), and set point (· · ·).

5.3 Robust behavior with OF control

To test the robustness of the OF controller, the reactor and the estimator initial states were deviated from the nominal open-loop unstable and maximum reaction rate steady-state, and subjected to the oscillatory feed concentration and temperature inputs

$$c_e = 0.99 + 0.01\cos(4\pi t), \quad T_e = 370 + 2\sin(4\pi t)$$

The constant errors in the estimation model correspond to: (i) $\hat{c}_e(t) = 0.991$, (ii) measured feed and reactor temperatures with considerable periodic error $\hat{T}_e(t) - T_e(t) = y(t) - T(t) = 2\cos(40\pi t)$ (four degrees amplitude band and frequency close to natural resonance mechanism), and (iii) -1.5, -10, and $+3$ % errors in the activation energy (γ), heat transfer coefficient (η), and adiabatic temperature rise (β), respectively. These errors represents a worst-case situation to subject the OF controller to a severe robustness test. The resulting closed-loop behavior is presented in Figure 3: (i) the reactor is adequately P-stable with a transient response trend that basically coincides with the one of the errorless model case (see Figure 2), (ii) as expected from the severe modelling errors, the unmeasured concentration exhibits a significant ($\approx -30\%$) asymptotic offset, some reaction rate offset ($\approx -20\%$) and the temperature estimate generated by the linear-dynamical advective (that is mass-energy balance based) estimation component yields an offset-less trend response, and (iii) given the flatness feature of the reaction kinetics in the isotonic branch of the reaction rate function, in spite of the -30% concentration trend offset, the reaction rate trend is only a -20% of its maximum set point value. Should it be necessary, the optimal rate offset can be reduced by online kinetic parameter model calibration on the basis of the occasional or periodic concentration measurements that are usually taken for quality monitoring purposes.

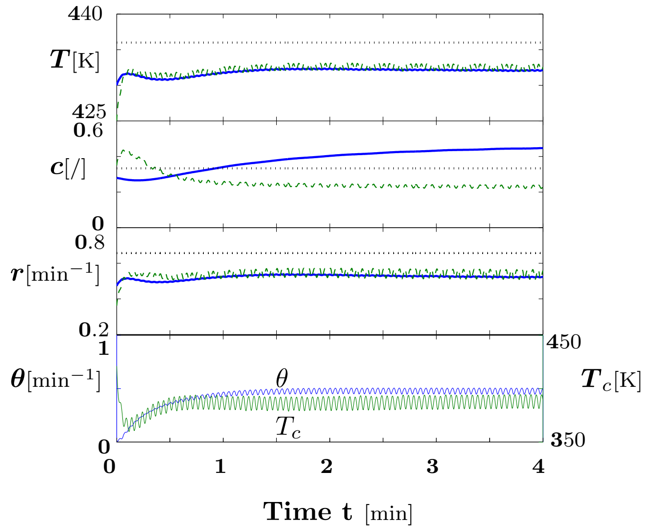

Fig. 3. Closed-loop robust behavior with nonlinear OF controller: input and response (—) , estimate (– –), and set point (· · ·).

5.4 Concluding Remarks

In agreement with the theoretically drawn methodology, the proposed passive-dissipative OF controller: (i) recovers rather well the behavior of its exact model-based nonlinear SF counterpart, with optimality-based robustness and control non-wastefulness, and (ii) exhibits P-(robust and non local) stability with respect to model, and measurement errors. The closed-loop behavior assessment through simulations made quantitative the P-stability features (like transient response speed, overshoot, high frequencies oscillatory components, and asymptotic response offsets), and verified the effectiveness of the gain tuning scheme obtained from the P-stability characterization.

6. CONCLUSIONS

A robust OF control design methodology for continuous reactors with temperature measurements has been presented. Structural (relative degree and global detectability) solvability conditions were identified and exploited to design a nonlinear dynamic dissipative-passive OF controller. The interlaced estimator-control design led to a robust OF control scheme with: (i) a systematic construction procedure, and (ii) a rigorous closed-loop (nonlinear-nonlocal) P-stability criterion, (iii) simple tuning guidelines, and (iv) behavior recovery, up to estimator convergence, of the exact model-based FF-SF nonlinear control. A Langmuir Hinshelwood kinetics (carbon monoxide oxidation) in an open-loop unstable reactor at maximum reaction rate was considered as a representative case example with numerical simulations.

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Appendix A. PROOF OF PROPOSITION 4.1

Recall the control (V) (13) and observer ($\hat{V}$) (20) storages, set the composed storage W, and write the corresponding dissipation ($\dot{W}$) along the closed-loop reactor motion:

$$W = V + \hat{V}, \quad \dot{W} = -z^T Q z, z = [e_c, \epsilon_c, e_T, \epsilon_T],$$

$$Q = \begin{bmatrix} k_c & -\iota_c(\theta_r + \varphi) & 0 & \kappa_r \varphi(c_e - c)/[2(c_e - \hat{c})] \\ \star & \theta_r + \varphi & (\beta\varphi)/2 & [\kappa_c - (\kappa_r + \beta)\varphi]/2 \\ \star & \star & k_T & 2\iota_1 + \iota_r \\ \star & \star & \star & \kappa_T + \iota_r \end{bmatrix}$$

$$\iota_c(k_c) = \frac{(\theta^* - [k_c - \varphi](c_e - c))^2}{4(c_e - \hat{c})(\theta_r + \varphi)}, \iota_r(\kappa_r) = \mu + \eta + \kappa_r \beta \varphi$$

$$\iota_T(k_c) = \frac{k_c \beta^2 \varphi^2}{4(\theta_r + \varphi)(k_c - \iota_c(k_c))}, \iota_1 = \frac{(k_T - \kappa_r \beta \varphi)^2}{4k_T} - \iota_r$$

$$\iota_2 = \frac{\varpi(k_c, \kappa_c, \kappa_r}{(\theta_r + \varphi)} - \iota_r, \quad \iota_\tau = \max\{\iota_1, \iota_2\},$$

and ϖ is a class-$\mathcal{K}$ function of its arguments. The enforcement of the positive defintness property in each of the four leading principal minors ($M_1, \ldots, M_4$), yields the conditions stated in Proposition 4.1, or equivalently the positive definitness of Q implying the closed-loop P-stability property. QED