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 ob-
tain the maximum product yield, these reactors must be operated at a steady-state with maxi-
mum reaction rate, a concentration that is not locally observable from a temperature measure-
ment. 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 concentra-
tion can be estimated and/or controlled. However, in the theoretical systems estimation liter-
ature 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 ad-
dressed in the present work; on whether it is possible to nonlocally control a continuous 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 feedforward, passivity and observ-
ability ideas yielded an output feedback cascade
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):

$$\begin{align*}
\dot{c} &= -\rho(c, T, p) + \theta(c_e - c) \\
\dot{T} &= \beta \rho(c, T, p) + \theta(T_e - T) - v(T - T_j) \\
y &= T, z_c = c, z_T = T, d_T = T_e, d_e = c_e
\end{align*}$$

Where $c$ is the reactant dimensionless concentration $T$ is the reactor temperature, $T_j$ is the jacket temperature, $\theta$ is the dilution rate, $v$ is the heat transfer coefficient, and $\beta$ 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 $\theta$ 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 ($dT$ and $dc_e$) 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,

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

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

$$0 = -\rho(\bar{c}, \bar{T}, p) + \theta(\bar{c}_e - \bar{c}), \quad \rho_c(\bar{c}, \bar{T}, p) = 0 \quad (3)$$

$$0 = \beta \rho(\bar{c}, \bar{T}, p) + \theta(\bar{T}_e - \bar{T}) - v(\bar{T} - \bar{T}_j)$$

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

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

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

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

$$\text{rank}[C] = 2 \iff v \neq 0, \bar{c}_e \neq \bar{c} ; \quad C = [B, AB]$$

$$\text{rank}[O] = 2 \iff \rho_c(c, T, p) \neq 0 ; \quad O = [c_y, c_yA]^T$$

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

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 $\rho(c, T, p) = [\dot{T} - \theta(\bar{c}_e - \bar{c}) - v(\bar{T} - \bar{T}_j)]/\beta$ 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 $\Omega$ (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 \((\theta)\) 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

\[
\begin{align*}
\dot{e}_c &= -k_c e_c,\quad e_c = c - \bar{c}
\end{align*}
\]

(4)

\[
\begin{align*}
\dot{e}_T &= -k_y e_T,\quad e_T = T - \bar{T}
\end{align*}
\]

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

\[
\theta = [-k_c (c - \bar{c}) + p(c, T, p)]/[e_c - c]
\]

(5)

\[
\begin{align*}
T_j = T + [-k_T (T - \bar{T}) - \beta p(c, T, p) - \theta (T_c - T)]/\nu
\end{align*}
\]

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 \((T, T_c)\) is measured, the feed concentration \((c_c)\) is nearly constant about its nominal value, and the thermodynamic-transfer parameter pair \((\beta, \nu)\) is reasonably known [in fact, \(\nu\) 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 \(\dot{\hat{c}}(t)\) of the reactor rate function \(\rho(c, T, t)\) 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

\[
\begin{align*}
\dot{T} &= \beta \dot{\hat{c}} + \theta (\dot{T_c} - \bar{T}) - \nu (\dot{T} - T_j) + 2\zeta \omega_T (y - \hat{T})
\end{align*}
\]

(6)

\[
\begin{align*}
\dot{\hat{c}} &= -\hat{r} + \theta (c_c - \bar{c}),\quad \hat{c}(0) = \hat{c}_0
\end{align*}
\]

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

\[
\begin{align*}
\hat{c}(t) - \bar{c}(t) \sim \hat{c}(t)
\end{align*}
\]

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

\[
\begin{align*}
\dot{\hat{c}} = -\hat{r} + \theta (c_c - \bar{c})
\end{align*}
\]

(8)

\[
\begin{align*}
\dot{T} = \beta \dot{\hat{c}} + \theta (\dot{T_c} - \bar{T}) - \nu (\dot{T} - T_j) + 2\zeta \omega_T (y - \hat{T})
\end{align*}
\]

(9)

\[
\begin{align*}
\hat{r} &= (\omega_T^2/\beta)(y - \bar{T})
\end{align*}
\]

(10)

\[
\begin{align*}
T_j &= T + [-k_T (\bar{T} - \bar{T}) - \beta \rho(c, T, p) - \theta (T_c - T)]/\nu
\end{align*}
\]

(11)

\[
\begin{align*}
\theta &= [-k_c (c - \bar{c}) + \hat{r}]/(\bar{c}_e - \bar{c})
\end{align*}
\]

(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 \(\theta\) proportionally to \(\hat{r}\) (Gonzalez and Alvarez, 2005).

3.3 Redesigned output-feedback controller

The preceeding 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 Luenberger-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 $\Omega$ (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

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

The corresponding passivated EKF is given by

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

$$
\dot{\hat{r}} = - 2\theta s + \nu - \rho^2(\hat{c}, \hat{T}, \hat{p}) s^2, \quad s(0) = 0
$$

$$
\dot{\hat{r}} = 0 \quad \hat{r} = \hat{r} - r, \quad \hat{c}_c = c - \hat{c}, \quad c_T = T - T, \quad \epsilon_c = \hat{c} - c.
$$

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

$$
g(c^+, \hat{T}, \hat{p}) > 0, \quad g(c < c^+, \hat{T}, \hat{p}) < 0
$$

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 $\Omega$ that lacks instantaneous nonlinear and linear (or) 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 redesign of OF controller:

$$
\dot{T} = \beta \hat{r} + \hat{\theta}(\hat{T}_c - \hat{T}) - \nu(\hat{T} - \bar{T}) + 2\zeta_T \omega_T (y - \bar{T})
$$

$$
\dot{\hat{r}} = (\omega_T^2 / \beta)(y - \bar{T})
$$

$$
\dot{\hat{c}} = -\hat{r} + \theta(\hat{c}_e - \hat{c}) + s p_c(\hat{c}, \hat{T}, \hat{p}) \left[ \hat{r} - \rho(\hat{c}, \hat{T}, \hat{p}) \right]
$$

$$
\dot{s} = -2\beta s + \nu - \rho^2(\hat{c}, \hat{T}, \hat{p}) s^2
$$

$$
\bar{T}_c = \bar{T} + [-k_T (\bar{T} - T) - \beta \hat{r} - \hat{\theta}(\hat{T}_c - \bar{T})] / \nu
$$

$$
\hat{\theta} = [-k_c(\hat{c} - \hat{c}) + \hat{r}] / (\hat{c}_e - \hat{c})
$$

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 $\Delta T_r, \Delta q_c, \Delta q_r, \Delta q_T, q_c, \lambda_c$ are defined on Appendix A):

$$
\dot{\hat{c}}_h = A_T \hat{r}_h + \hat{q}_c_h \left( c, T, r, c_e, T_e, k_c, k_T, \epsilon_c, \epsilon_e, \epsilon_T, \hat{r}_e \right) \quad (15)
$$

$$
\dot{s} = -2s + q_c(c, T, \nu, s, c_e) \quad (16)
$$

$$
\dot{\epsilon}_c = -k_c c + q_c(c, T, r, c_e, \nu, c_e, \bar{p}, \epsilon_e) \quad (17)
$$

$$
\dot{\epsilon}_T = -k_T \epsilon_T + q_T(k_c, k_T, \epsilon_c, \bar{p}, \epsilon_e, \bar{\epsilon}_e) \quad (18)
$$

$$
\epsilon_c = -k_c c + q_c(k_c, k_T, \epsilon_c, \bar{p}, \epsilon_e, \bar{\epsilon}_e) \quad (19)
$$

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

the perturbation terms vanish as follows:

$$
q_c(c, T, r, c_e, T_e, k_c, k_T; 0, 0, 0, 0, 0) = 0
$$

$$
q_c(c, T, r, c_e, T_e, k_c, k_T; 0, 0, 0, 0, 0) = 0
$$

$$
q_T(k_c, k_T; 0, 0, 0, 0, 0) = 0
$$

$$
q_c(k_c, k_T; 0, 0, 0, 0, 0) = 0
$$

$$
q_c(c, T, \nu, s; 0) = 0
$$

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 Ricatti 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 $(\nu, \omega_T)$ gains $(\nu^T = 1.5)$ are chosen so that the following low and high gain conditions are met:

(i) $k_c, k_T > 0$, $\nu^-(k_c) < \nu < \nu^+(k_c)$

(ii) $\omega_T^-(k_c, k_T) < \omega_T < \omega_T^+(k_c, k_T)$

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 $\nu$ (or $\omega_T$) 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 $\nu^-$ and $\omega_T^-$ (or $\nu^+$ and $\omega_T^+$) 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, \( \omega_T \approx 3k_T \), \( \nu \approx \frac{3k_c}{\beta} \).

2. Increase \( \omega_T \) and \( \nu \) 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:

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

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 \( \theta \) (or \( T_j \)) is constrained to take values in \([0.1, 1.2] \) \( \text{or} \) \([300, 500]\))).

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 \( \bar{x} \) \( (T_0 \epsilon [416, 456], c_0 \epsilon [0.1, 0.39]) \), (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 \( T_0 = T + 6 \) 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

<table>
<thead>
<tr>
<th>( k = e^{-\gamma} \cdot \gamma = 1064, \sigma = 3, \theta = 0.989 )</th>
<th>( \nu = c_e = 1, T_0 = T_j = 370, \beta = 200 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>steady states</td>
<td>( S_I )</td>
</tr>
<tr>
<td>concentration [mol/L]</td>
<td>0.991</td>
</tr>
<tr>
<td>temperature [K]</td>
<td>370.88</td>
</tr>
<tr>
<td>local condition</td>
<td>stable</td>
</tr>
</tbody>
</table>

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

\[
A_{\tau,r} = \begin{bmatrix}
-k_T - 2\zeta_T \omega_T & \beta \\
0 & -\omega_T^2/\beta
\end{bmatrix}, \quad \lambda_c = k_c \left(1 + \frac{1}{c_e - c}\right) + \beta \sec^\theta
\]

| sec^\theta = \rho(c + \bar{c}, T, p) - \rho(c, T, p), \\ q_{\bar{c}} = [q_T, q_r]^T |
|---|---|
| \( q_T = (T - T_0) (\bar{\theta} - \theta) + \gamma (\bar{T}_j - T_j) \) |
| \( q_r = p_c(T, p) k_c(e_e + \bar{c}) \) |
| \( q_e = \bar{c} + \bar{r} + (\bar{\theta} - \theta) (\bar{c}_e - \bar{c}) \) |
| \( q_{c_e} = -\bar{g}(\bar{c}, \bar{T}, \bar{v}) \left[ \rho(c, T, p) \right] - \bar{c} - (\bar{c}_e - \bar{c}) \) |
| \( q_{c_e} = \bar{r} + (\bar{\theta} - \theta) \left( T_0 - T_j \right) - \bar{c} (\bar{T}_j - T_0) \) |

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

\[
\dot{x} = f(x, u), \quad f(0,0) = 0 \quad (B.1)
\]

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 \( \lambda_x^u \) .
Theorem 2. (Small gain) (Isidori, 1995) Consider two IS stable systems (with convergence parameters \( \lambda_x \) and \( \lambda_y \)) \( \dot{x} = f(x, y, u) \lambda_x \) \( \dot{y} = g(x, y, u) \lambda_y \) The interconnection of the systems is IS stable if:
\[
(a_x L^f_x / (a_y L^g_y)) < 1
\]
where \( L^f_x \) 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

REFERENCES


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


