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PI-inventory control of continuos chemical reactors with non-monotonic kinetics.

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Abstract— In this work, the problem of controlling a continuos jacketed chemical reactor with temperature measurements and non-monotonic reaction rate is addressed. The reactor must operate about a (possibly open-loop unstable) steady-state where the reaction rate is maximum with respect to concentration and there is lack of local observability. The combination of nonlinear constructive and (PI and inventory) industrial control ideas, in the light of system characteristics, yields a control scheme with: (i) linear-decentralized PI volume control, (ii) linear-decentralized PI cascade temperature control, (iii) a ratio-type dynamic material-balance concentration controller driven by the integral actions of the primary and secondary loops of the temperature controller, and (iv) easy-to-apply tuning guidelines coupled to a nonlocal IS stability criterion. The proposed approach is tested with a representative case example.

Keywords: Reactor Control, Process Control, PI Controllers.

I. Introduction

An important class of chemical and biological reactors has non-monotonic kinetic rate dependency on concentration, and due to this, exhibit nonlinear behavior, including multiplicity, stable and unstable critical points, limit cycling, and parametric sensitivity [1], [2], [3]. The reactor must be designed to operate about a (possibly open-loop unstable) steady-state with maximum reaction rate (i.e. productivity) and lack of local obsevability [12].

Hitherto, the reactor control problem has been addressed with a diversity of procedures that lack systematization and formal closed-loop stability assesments. Recently, the problem has been addressed with approaches that exploit structural (relative degree and zero dynamics) detectability properties to drawn a control scheme with (i) a decoupled passive temperature controller that on-line quickly estimates the reaction rate and manipulates the jacket temperature, and (ii) a material balance controller that is driven by the reaction rate estimate and estimates the unmeasured concentration by on-line integrating the dynamic mass balance [10] or by a mass balance in conjunction with an EKF that speeds up the concentration estimate convergence rate [11]. The last concentration estimator has a passivated structure in the sense that the heat balance-based reaction rate estimate is regarded as a virtual measurement for the EKF concentration estimator.

However the implementation of this control has some drawbacks for industrial applicability: (i) the control scheme is considerably more complex and model dependent than the ones (linear PI and ratio controllers) commonly used in industry, (ii) the volume and jacket temperature control components are not included, in the undestanding that the jacket coolant rate is the actual manipulated variable for temperature control, and (iii) there is a lack of formal stability assessments with tractable (i.e., conventional-like) tuning guidelines. From an industrial reactor control perspective these drawbacks signify serious complexity, reliability, maintenance and cost concerns.

In this work the problem of controlling a continuous exothermic chemical reactor with non-monotonic reaction rate, using volume and temperature measurements, about a possibly (open-loop unstable) steady-state with maximum productivity and lack of local observability is addressed. We are interested in a robust control design in the light of a nonlocal inpu-to-state stability framework. For applicability purposes, we are interested in a control scheme with: (i) maximum linearity, decentralization and model independency features, and (ii) a systematic construction procedure.

First, the preceding two-state (concentration-temperature) dynamics (1a,1b) is augmented with the ones of the jacket and volume. Then, the temperature is controlled by means of a linear cascade controller with conventional-like linear PI loops, and the integral action of the loops in conjunction with the mass-energy balances provide an estimate of the reaction rate. Then, the reaction rate is regarded as a virtual measurement to draw a concentration estimate from a single state EKF built accordingly to the dynamic mass balance. The volume is controlled with a standard-linear PI controller. The approach is tested with a case example through simulations.

II. Control Problem

Consider a continuous chemical reactor (depicted in Fig.1) where an exotermic reaction takes place.

From standard mass and energy conservation argu-

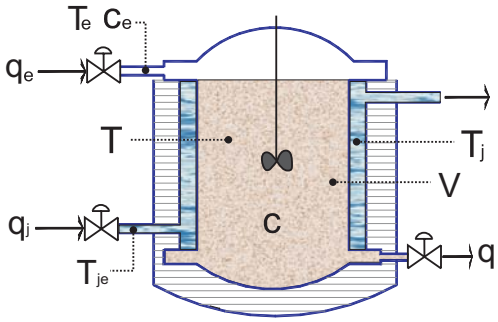

Figure 1. Jacketed Continuous Stirred Tank Reactor

ments the reactor model is given by :

$$\begin{aligned}
\dot{c} &= -\rho(c,T,p) + \frac{q_e}{V}(c_e - c) = f_c && \text{(1a)}\\
\dot{T} &= \beta\rho(c,T,p) + \frac{q_e}{V}(T_e - T) - \upsilon(T - T_j) = f_T && \text{(1b)}\\
\dot{T}_j &= \alpha_j\upsilon(T - T_j) + \alpha_q q_j(T_{je} - T_j) = f_j && \text{(1c)}\\
\dot{V} &= q_e - q = f_V && \text{(1d)}\\
z_c &= c, \;\; z_T = T, \;\; z_V = V && \text{(1e)}\\
y_T &= T, \;\; y_j = T_j, \;\; y_V = V && \text{(1f)}
\end{aligned}$$

Where (υ) {or $(\alpha_j\upsilon)$} is the heat transfer coefficient divided by the reactor {or cooling system} heat capacity, (β) is the adiabatic temperature rise (i.e., the heat of reaction divided by the reactor heat capacity), (α_q) is the product of the coolant density and specific heat capacity divided by the heat capacity of the cooling system, and (c_e) {or T_e} is the feed concentration {or temperature}. The states are the reactant dimensionless concentration (c) referred to a given value, the reactor temperature (T), the jacket temperature (T_j) and the reactor volume (V), the control inputs are the input (q_e) and output (q) flows and the coolant entrance flow (q_j), the regulated outputs are the concentration (c) the temperature (T) and the volume (V), the measured outputs are the volume (V) and the reactor (T) and jacket (T_j) temperatures, the exogenous inputs are the measured reactor (T_e) and jacket (T_{je}) feed temperatures, and the concentration (c_e) that is not measured, but a nominal value is known.

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:

$$\Omega = \{\mathbf{x} \in \mathrm{X} \mid \rho_c(c,T,p) := \frac{\partial\rho(c,T,p)}{\partial c} = 0\} \qquad (2)$$

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

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

A previuos analysis [11] shows that the related observability matrix of the linear reactor approximation is singular in the curve Ω, meaning that the reactor is not locally instantaneously observable at Ω [4].

Due to conservation principles, second law of thermodynamics, and operation constraints the following inequalities are met:

$$\begin{aligned}
c_e^- &\le c_e \le 1, \;\; T_e^- \le T_e \le T_e^+, \;\; T_{je}^- \le T_{je} \le T_{je}^+\\
q_e^- &\le q_e \le q_e^+, \;\; q^- \le q \le q^+ \implies 0 < c < 1\\
T_j^- &< T_j < T_j^+, \;\; V^- < V < V^+
\end{aligned}$$

$$\min(T_j^-, T_e^-) = T^- < T < T^+ = \max(T_j^+, T_e^+)$$

In vector compact notation, the reactor system (1) is written as follows

$$\begin{aligned}
\dot{\mathbf{x}} &= f(\mathbf{x},\mathbf{u},\mathbf{d}) \;\; , && \mathbf{x}(0) = \mathbf{x}_0 \qquad (3)\\
\mathbf{y} &= C_y\mathbf{x} \;\; , && \mathbf{z} = C_z\mathbf{x}
\end{aligned}$$

where $\mathbf{x}$ is the state, $\mathbf{u}$ is the control input, $\mathbf{z}$ is the regulated output, $\mathbf{y}$ is the measured output, $\mathbf{d}$ is the exogenous input, and

$$\begin{aligned}
\mathbf{d} &= \begin{bmatrix} T_e \\ T_{je} \\ c_e \end{bmatrix} \in D, \mathbf{u} = \begin{bmatrix} q_e \\ q \\ q_j \end{bmatrix} \in U, \mathbf{x} = \begin{bmatrix} c \\ T \\ T_j \\ V \end{bmatrix} \in X,\\
\mathbf{y} &= [T, T_j, V]^T \in Y, \qquad \mathbf{z} = [c, T, V]^T \in Z
\end{aligned}$$

$$(y_1, y_2, y_3)^T = C_y x, \qquad (z_1, z_2, z_3)^T = C_z x$$

The steady-state operation

$$f(\bar{\mathbf{x}}, \bar{\mathbf{u}}, \bar{\mathbf{d}}) = 0, \qquad \bar{\mathbf{y}} = C_y\bar{\mathbf{x}}, \qquad \bar{\mathbf{z}} = C_z\bar{\mathbf{x}}$$

may have multiple steady states $\bar{\mathbf{x}} = \bar{\mathbf{x}}_1, ...\bar{\mathbf{x}}_{n_s}$ and the process design problem is to choose the reactor dimensions and operation conditions so that $\bar{\mathbf{x}} \in \Omega$ in order to obtain maximum productivity.

The control problem consists in given a steady-state operation $(\bar{\mathbf{x}}, \bar{\mathbf{u}}, \bar{\mathbf{d}}) = 0$, designing a controller that, driven by measurements $\mathbf{y}$ and $\mathbf{d}$, manipulates the control $\mathbf{u}$ to regulate the output $\mathbf{z}$ about $\bar{\mathbf{z}}$ with closed-loop state stability. This is

$$\mathbf{x}_0 \in \mathrm{X}_0, c_e \in \mathrm{X}_{c_e}, T_e \in \mathrm{X}_{T_e}, T_{je} \in \mathrm{X}_{T_{je}} \implies z \to \bar{z}, x \to \bar{x}$$

meaning stability in a practical sense (admissible-size disturbances produce admissible-size state and output deviations).

III. Passivity-based Control design

The application of the nonlinear geometric technique [13] to our problem yields that: (i) the static SF control problem is not solvable because there is not relative degree vector, and (ii) the problem is solvable with dynamic SF control, with dynamic extension for the exit flow rate, and relative degree vector= $[1,2,1]$. To remove the high relative degree obstacle for control

robustness [5] the control is redesigned by passivation by backstepping with emphasis in the attainment of linearity, decentralization and model independency applicability-oriented features [10].

A. State Feedback Control

Recall the reactor model (1), assume the state ($\mathbf{x}$) and exogenous inputs ($\mathbf{d}$) are known, regard T_j^* as a virtual control input, enforce the closed-loop (primary) regulation dynamics

$$\begin{aligned} \dot{e}_T &= -k_T e_T, \quad \dot{e}_c = -k_c e_c, \quad \dot{e}_V = -k_V e_V \quad (4) \\ e_T &= T - \bar{T}, \quad e_c = c - \bar{c}, \quad e_V = V - \bar{V} \quad (5) \end{aligned}$$

combine these equations with (1a,1b,1d) and solve the resulting equations for (q_e, q, T_j^*) to obtain the primary controller

$$\begin{aligned} q_e &= V[-k_c(c-\bar{c}) + \rho(c,T,p)]/\,(c_e - c) \quad (6a) \\ q &= -k_V(V-\bar{V}) + q_e \quad (6b) \\ T_j^* &= \frac{-k_T(T-\bar{T}) - \beta\rho(c,T,p) - \frac{q_e}{V}(T_e - T) + \upsilon T}{\upsilon} \quad (6c) \end{aligned}$$

Enforce the closed-loop regulation dynamics

$$\dot{e}_j = -k_j e_j, \quad e_j = T_j - T_j^* \quad (7)$$

combine this equation with (1c), solve the resulting equation for q_j to obtain the secondary temperature controller

$$\begin{aligned} q_j &= \frac{\dot{T}_j^* - k_j(T_j - T_j^*) - \alpha_j \upsilon (T - T_j)}{\alpha_q(T_{je} - T_j)} \quad (8a) \\ \dot{T}_j^* &= \frac{1}{\upsilon}\left[-k_T\dot{T} - \beta\left(\rho_c\dot{c} + \rho_T\dot{T}\right)\right] \\ &\quad -\frac{q_e}{\upsilon}\left(\frac{(\dot{T}_e - \dot{T})V - \dot{V}(T_e - T)}{V^2}\right) + \dot{T} \quad (8b) \end{aligned}$$

where the last equation follows from the analytic derivation of (6c). The closed loop behavior of this SF controller (6,8) constitutes the target to be recovered with an output feedback (OF) controller.

B. Output Feedback Control

Since the concentration-temperature pair is not locally observable at the curve Ω, a nonlinear high-gain Luenberguer observer cannot be employed. Instead an EKF (9) is employed to obtain a joint concentration-temperature $(\hat{c}, \hat{T})$ observation structure [9]. The combination of this EKF with the passivated SF controller (6,8) yields the OF controller.

$$\begin{aligned} \dot{\hat{c}} &= -\rho(\hat{c},\hat{T},p) + [q_e(c_e - \hat{c})]/y_V + \frac{\sigma_{12}}{r_{11}}\left(y_T - \hat{T}\right) \quad (9a) \\ \dot{\hat{T}} &= \beta\rho(\hat{c},\hat{T},p) + [q_e(T_e - \hat{T})]/y_V - \upsilon(\hat{T} - T_j) \\ &\quad + \frac{\sigma_{22}}{r_{11}}\left(y_T - \hat{T}\right) \quad (9b) \\ \dot{\sigma}_{11} &= 2\big[(-\rho_c(\hat{c},\hat{T},p) + \frac{q_e}{y_V})\sigma_{11} - \rho_T(\hat{c},\hat{T},p)\sigma_{12}\big] \\ &\quad + q_{11} - \frac{\sigma_{12}^2}{r_{11}} \quad (9c) \\ \dot{\sigma}_{22} &= 2\big[\beta\rho_c(\hat{c},\hat{T},p)\sigma_{12} + (\beta\rho_T(\hat{c},\hat{T},p) - \frac{q_e}{y_V} - \upsilon)\sigma_{22}\big] \\ &\quad + q_{22} - \frac{\sigma_{22}^2}{r_{11}} \quad (9d) \\ \dot{\sigma}_{12} &= \beta\sigma\rho_c(\hat{c},\hat{T},p)_{11} + [-\rho_c(\hat{c},\hat{T},p) + \frac{q_e}{y_V} + \beta\rho_T(\hat{c},\hat{T},p) \\ &\quad -\frac{q_e}{y_V} - \upsilon]\sigma_{12} - \rho_T(\hat{c},\hat{T},p)\sigma_{22} - \frac{\sigma_{12}\sigma_{22}}{r_{11}} + q_{21} \quad (9e) \end{aligned}$$

$$\begin{aligned} q_e &= y_V(-k_c(\hat{c} - \bar{c})) + \rho(\hat{c},\hat{T},p)/\,(c_e - \hat{c}) \quad (10a) \\ q &= -k_V(y_V - \bar{V}) + q_e \quad (10b) \\ Tj^* &= \frac{-k_T(y_T - \bar{T}) - \beta\rho(\hat{c},\hat{T},p) - \frac{q_e}{V}(T_e - y_T) + \upsilon y_T}{\upsilon} \quad (10c) \\ q_j &= \frac{\dot{T}_j^* + (-k_j(y_j - T_j^*) - \alpha_j\upsilon(y_T - y_j)}{\alpha_q(T_{je} - y_j)} \quad (10d) \\ \dot{T}_j^* &= \frac{1}{\upsilon}\left[-k_T\dot{T} - \beta\left(\rho_c\dot{c} + \rho_T\dot{T}\right)\right] \\ &\quad -\frac{q_e}{\upsilon}\left(\frac{(\dot{T}_e - \dot{T})V - \dot{V}(T_e - T)}{V^2}\right) + \dot{T} \quad (10e) \end{aligned}$$

where $\rho_T(c,T,p) := \frac{\partial\rho(c,T,p)}{\partial T}$.

As it can be seen, the OF controller consists in 5 ordinary differential equations (ODE's) and 5 algebraic equations (AE's), the construction of the controller needs the reaction rate function $\rho(c,T,p)$, its partial derivatives respect to T and c, its parameter vector p, as well as the heat transfer coefficient υ.

IV. Redesigned Control

From an industrial reactor control perspective the OF controller (9,10) is very complex and model dependent in relation to the industrial standard linear (P or PI) controllers. Thus in this section the controller is redesigned with an applicability-oriented linearity, decentralization and model independence features.

A. State Feedback Control

Let us rewrite the reactor model (1) in a parametric form [10] with a static a_T, a_j, a_V and a synthetic b_T, b_j, b_V load disturbances

$$\begin{aligned} \dot{T} &= a_T T_j + b_T, \qquad y_T = T \quad (11a) \\ \dot{T}_j &= a_j q_j + b_j, \qquad y_j = T_j \quad (11b) \\ \dot{V} &= a_V q + b_V, \qquad y_V = V \quad (11c) \end{aligned}$$

$$\begin{aligned} b_T &= \beta_T(c,T,T_j,V,T_e,q_e) \quad (12a) \\ b_j &= \beta_j(T,T_j,T_{je},q_j) \quad (12b) \\ b_V &= \beta_V(q_e) \quad (12c) \end{aligned}$$

$$\dot{c} = -\rho(c,T,p) + \frac{q_e}{V}(c_e - c), \qquad z_c = c \quad (13)$$

where $a_T = \bar{\upsilon}, \quad a_j = \bar{\alpha}_j(\bar{T}_{je} - \bar{T}_j), a_V = -1$
$\bar{\upsilon}, \bar{\alpha}_j, \bar{T}_{je}, \bar{T}_j$ are approximations of the steady-state values of each variable or parameter, and

$$\begin{aligned} \beta_T &= \beta\rho(c,T,p) + (q_e/V)(T_e - T) - \upsilon(T - T_j) - a_T T_j \\ \beta_j &= \upsilon_j(T - T_j) + q_j\alpha_j(T_{je} - T_j) - a_j q_j, \quad \beta_V = q_e \end{aligned}$$

This representation of the reactor has a linear and decentralized dynamical component (11), and interactive non linear dynamical (13) and static (12) components. Assume the the load disturbances are known, enforce the closed-loop dynamics (4) to the reactor parametric form (11) obtaining

$$\begin{aligned} q &= (-k_V(V - \bar{V}) - b_V)/(a_V) && (14a) \\ Tj^* &= (-k_T(T - \bar{T}) - b_T)/(a_T) && (14b) \\ q_j &= (\dot{T}_j^* - k_j(T_j - Tj^*) - b_j)/(a_j) && (14c) \end{aligned}$$

This passive SF controller constitutes a linear and reduced model dependency version of the cascade temperature and volume controllers (6), but still needs an extra high model dependent equation that follows from the analytic derivation of (14b)

$$\dot{T}_j^* = \iota(\dot{T}, \dot{b}_T) \quad (15)$$

Enforce the closed-loop dynamics (7) to the reactor concentration component (13) and obtain the concentration SF controller.

$$q_e = \frac{y_V\left(-k_c(c - \bar{c}) + \rho(c,T,p)\right)}{(c_e - c)} \quad (16)$$

B. Output-Feedback Control

The linear and decentralized dynamical component (11) of the reactor can be expressed as follows:

$$\begin{aligned} \dot{x}_\iota &= a_\iota u_\iota + b_\iota,\ y_\iota = x_\iota, \quad \iota = V,T,j \\ u_V &= q, \quad u_T = T_j, \quad u_j = q_j \end{aligned}$$

Each synthetic load is determined by the input-output pair $b_\iota = \dot{x}_\iota - a_\iota u_\iota$, so it can be quickly reconstructed by a set of reduced order observers [8]

$$\begin{aligned} \dot{\chi}_\iota &= -\omega_\iota\chi_\iota - \omega_\iota^2 y_\iota - \omega_\iota a_\iota u_\iota, \ \ \chi_\iota(0) = -\omega_\iota y_{\iota 0} && (17) \\ \hat{b}_\iota &= \chi_\iota + \omega_\iota y_\iota \\ \iota &= V,T,j \end{aligned}$$

Combining this decentralized set of filters with the SF temperature and volume controllers (6) a set of linear and decentralized OF controllers is obtained:

$$\begin{aligned} \dot{\chi}_\iota &= -\omega_\iota\chi_\iota - \omega_\iota^2 y_\iota - \omega_\iota a_\iota u_\iota, \ \ \chi_\iota(0) = -\omega_\iota y_{\iota 0} && (18a) \\ u_\iota &= \left(\dot{\bar{y}}_\iota - k_\iota(y_\iota - \bar{y}_\iota) - \chi_\iota - \omega_\iota y_\iota\right)/(a_\iota) && (18b) \end{aligned}$$

where in classical PI form are written as follows:

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

where the proportional and integral gains are functions of estimation ω_ι and control k_ι gains.

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

Once the synthetic loads are estimated the derivative of the virtual set point $\dot{T}_j^*$ follows from the time derivative of (14b) and the sustitution of b_T by its estimate $\hat{b}_T$

$$\dot{T}_j^* = -k_T T_j - \frac{k_T}{a_T}\chi_T - \frac{k_T\omega_T}{a_T}T \quad (19)$$

Also from $\hat{b}_T$ and $\hat{b}_j$ the instantaneous value of the heat exchange coefficient ($\hat{\upsilon}$) and the reaction generation rate ($\hat{r}$) can be recovered by solving two algebraic equations:

$$\begin{aligned} \hat{\upsilon} &= \frac{\chi_j + \omega_j T_j - \left(\alpha_q q_j(T_{je} - T_j) + a_j q_j\right)/(T - T_j)}{\alpha_j} && (20a) \\ \hat{r} &= \frac{\chi_T + \omega_T y_T - \frac{q_e}{V}(T_e - T) + \hat{\upsilon}(T - T_j) + a_T T_j}{\beta} && (20b) \end{aligned}$$

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 degree (say two) obstacle [5], regard the reaction rate estimate $\hat{r}$ (20b) as a virtual measurement for the concentration dynamics [11], according to the expressions

$$\dot{c} = -\hat{r} + q_e(c_e - c)/V, \qquad \hat{r} = \rho(c,T,p)$$

and the corresponding EKF is

$$\begin{aligned} \dot{\hat{c}} &= -\hat{r} + \frac{q_e}{V}(c_e - \hat{c}) + s\rho_c(\hat{c},\hat{T},p)\left[\hat{r} - \rho(\hat{c},\hat{T},p)\right] && (21a) \\ \dot{s} &= -2sq_e/V + \nu - \rho_c^2(\hat{c},\hat{T},p)s^2, \quad s(0) = s_0 && (21b) \\ s &= \sigma/q_r, \ \ \nu = q_c/q_r \end{aligned}$$

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

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

These vanishing-gain switching properties implies that the estimator injection ceases as the reactor approaches the curve Ω that lacks local observability or, equivalently, the estimator behaves in open-loop regime. It has to been mentioned that in spite of the needing of the reaction rate function and its partial derivative respect to concentration in fact the model dependency is minimal because the EKF estimator only needs a tendency-like approximation of the reaction

rate function. The combination of the concentration SF controller (16) and EKF (21) with the reaction rate and heat transfer coefficient estimators (20), and the set of linear controllers (18) yields the OF controller

Temperature

$$\dot{\chi}_T = -\omega_T \chi_T - \omega_T^2 y_T - \omega_T a_T T_j^* \quad (22a)$$

$$Tj^* = \left(-k_T(y_T - \bar{T}) - \chi_T - \omega_T y_T\right)/(a_T) \quad (22b)$$

$$\dot{\chi}_j = -\omega_j \chi_j - \omega_j^2 y_j - \omega_j a_j q_j \quad (22c)$$

$$q_j = \left(\dot{T}_j^* - k_j(y_j - Tj^*) - \chi_j - \omega_j y_j\right)/(a_j) \quad (22d)$$

$$\dot{T}_j^* = -k_T T_j - \frac{k_T}{a_T}\chi_T - \frac{k_T \omega_T}{a_T} T \quad (22e)$$

Volume

$$\dot{\chi}_V = -\omega_V \chi_V - \omega_V^2 y_V - \omega_V a_V q \quad (23a)$$

$$q = \left(-k_V(y_V - \bar{V}) - \chi_V - \omega_V y_V\right)/(a_V) \quad (23b)$$

Concentration

$$q_e = \frac{y_V\left(-k_c(\hat{c} - \bar{c}) + \hat{r}\right)}{(c_e - \hat{c})} \quad (24a)$$

$$\hat{r} = [\chi_T + \omega_T y_T - \frac{q_e}{V}(T_e - y_T) + \frac{1}{\alpha_j}(\chi_j + \omega_j y_j - \alpha_q q_j (T_{je} - y_j) + a_j q_j) + a_T y_j]/\beta \quad (24b)$$

$$\dot{\hat{c}} = -\hat{r} + \frac{q_e}{y_V}(c_e - \hat{c}) + s\rho_c(\hat{c}, T, p)\left[\hat{r} - \rho(\hat{c}, T, p)\right] \quad (24c)$$

$$\dot{s} = -2sq_e/y_V + \nu - \rho_c^2(\hat{c}, T, p)s^2 \quad (24d)$$

As it can be seen this redesigned OF controller consists in 5 ODE's and 6 AE's and resembles industrial conventional temperature and volume control components. An additional algebraic equation (24b) is needed to recover the instantaneous value of the reaction rate that is used in the control and estimation of concentration. Notice also that for the concentration estimate is only needed a tendency-like approximation of the reaction rate function that acts as a accelerator of the concentration estimation with respect the open loop regime [10], meaning that there is a model independency not found in the OF controller (9,10).

C. Closed loop stability

The application of the OF controller (22,23,24) to the chemical reactor (1) yields the closed-loop dynamics

$$\dot{e}_c = -k_c e_c + q_c(c, T, T_j, V, T_e, T_{je}, c_e, s, b_T, b_j; \epsilon_T, \epsilon_j, \epsilon_c) \quad (25a)$$

$$\dot{e}_T = -k_T e_T + q_T(T, b_T; \epsilon_T) \quad (25b)$$

$$\dot{e}_j = -k_j e_j + q_j(T, T_j, b_T, b_j; \epsilon_T, \epsilon_j) \quad (25c)$$

$$\dot{e}_V = -k_V e_V + q_V(V, b_V; \epsilon_V) \quad (25d)$$

$$\dot{\epsilon}_T = -\omega_T \epsilon_T + (\ddot{T} - a_T \dot{T}_j) \quad (26a)$$

$$\dot{\epsilon}_j = -\omega_j \epsilon_j + (\ddot{T}_j - a_j \dot{q}_j) \quad (26b)$$

$$\dot{\epsilon}_V = -\omega_V \epsilon_V + (\ddot{V} - a_V \dot{q}) \quad (26c)$$

$$\dot{\epsilon}_c = -k_c \epsilon_c - s\rho_c(\hat{c}, T)\left[\hat{r} - \rho(\hat{c}, T)\right] \quad (26d)$$

$$\dot{s} = \frac{-2s}{c_e - \hat{c}}\left[-k_c(e_c - \epsilon_c) + \hat{r}\right] + \nu - s^2 \rho_c(\hat{c}, T) \quad (26e)$$

where: $e_c = c - \bar{c}, e_T = T - \bar{T}, e_V = V - \bar{V}, e_j = T_j - T_j^*, \epsilon_c = c - \hat{c}, \epsilon_T = b_T - \hat{b}_T, \epsilon_j = b_j - \hat{b}_j, \epsilon_V = b_V - \hat{b}_V$.

Subsistem (25) without estimation errors ($\epsilon_i = 0$) constitutes the reactor closed-loop dynamics with SF control (6,8), and subsystem (26) represents the IS-stable estimator dynamics in closed-loop mode. The closed-loop system is the interconnection of quickly varying error dynamics (26a-26c), slowly varying estimation error dynamics (26d,26e), and slow closed-loop dynamics (25). In the case of monotonic kinetics, the closed-loop stability conditions can be drawn by applying standard small-gain [10] or direct Lyapunov methods [14]. Thus, the application of the same approach can be applied to asses the closed-loop stability of our system (25-26), with one important consideration: the non monotonic feature of the reactor and the presence of the Ricatti equation (26e). The formal stability proof is underway.

TABLE I

Steady states for operation conditions

$k = e^{25}, \gamma = 1e4, \sigma = 3, \upsilon = c_e = \alpha_q = 1, T_e = T_j = 370$ $\beta = 200, \alpha_j = 10, q_e = q = 0.989, q_j = 8.685, T_{je} = 293$			
steady states	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

V. Application example

The representative example was built recalling the non-monotonic kinetic dependency form from a previously reported experimental study for a catalytic reactor where carbon monoxide was burned to yield carbon dioxide [6], and modify it to draw a case where the unstable steady state coincided with the point that yielded the maximum reaction rate at a prescribed temperature. The non-monotonic kinetics is given by:

$$\rho(c, T, p) = \left(cke^{-\left(\frac{\gamma}{T}\right)}\right)/\left(1 + \sigma c\right)^2 [mol/L \cdot \min] \quad (27)$$

For the operation conditions listed in Table I, there are three steady-states, two stable ones S_I (ignition) and S_E (extinction) and one unstable (U).

To represent a realistic situation, the control signals are constrained heuristically to [0,4],[0,4] and [0,20] for q, q_e and q_j respectively. The gains were choosed to achieve a sufficient dynamic separation as: $\omega_j = 20$, $k_j = 6$, $\omega_T = 50$, $k_T = 3$, $\omega_V = 50$, $k_V = 3$, $\nu = 1$ and $k_c = 2$. The initial conditions were $x(0) = [0.2, 430, 365, 0.9]^T, \hat{c}(0) = 0.25, \sigma(0) = 0, \chi_j(0) = -\omega_j Tj(0), \chi_T(0) = -\omega_T T(0), \chi_V(0) = -\omega_V V(0)$. The simulation results can be seen in Fig. 2. Other simulation was done to compare the original (9,10) and redisegnided PI-inventory (22,24,23) OF controllers behavior. The same control gains were used in both controllers. For the EKF the next values were taken from [6] where a minimum least-squares criterion was used with experimental data from a catalytic reactor: $q_{11} = 7.590 \times 10^{-3}, q_{22} = 6.006 \times 10^{-7}, q_{21} = 0, r_{11} = 2.376 \times 10^{-7}$ and additionally $\sigma_{nn}(0) = 0, \hat{T}(0) = 440$.

It can be noticed that, in this case, the redesigned PI-inventory controller has the same performance with respect the more complex (and model dependent) OF passive controller. A last simulation was made to compare the robustness of both approaches. The reaction rate was modified with the next typical parameter errors [10]: -9.5% in the pre-exponential factor k, -0.5% in the adsorption constant σ and -6.6% in the activation energy γ. The results show that the redesigned PI-inventory controller has a more robust behavior with respect to the OF passive controller.

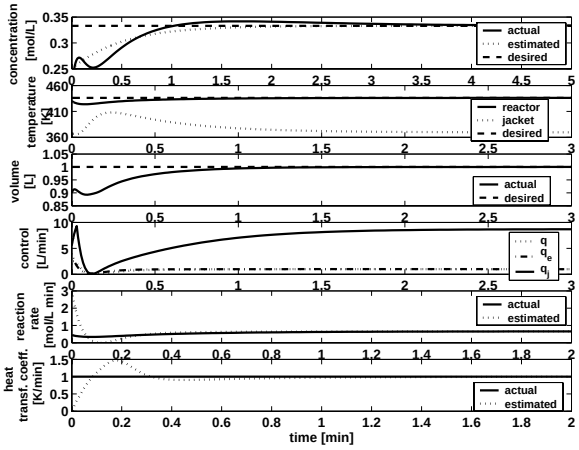

Figure 2. Closed-loop behavior with PI-inventory controller

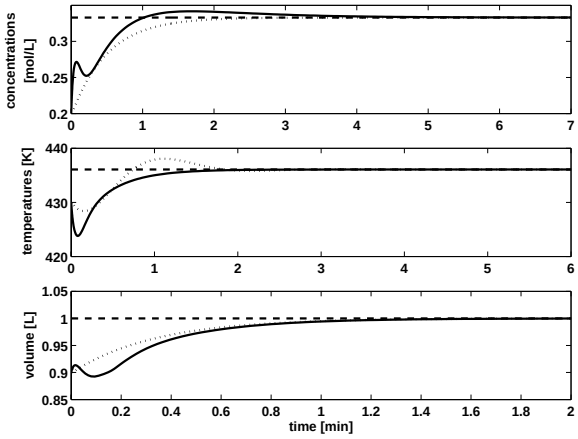

Figure 3. Closed-loop behavior with (9,10) nonlinear passivated OF (..) and (22,23,24) PI-inventory OF (-) control.

VI. Conclusions

The problem of controlling a continuos jacketed chemical reactor with temperature measurements and non-monotonic reaction rate was addressed, considerying a complete model with four states. The combination of nonlinear constructive and (PI, and inventory) industrial control approaches yielded a control scheme with linear-decentralized PI cascade temperature and volume controls, and a ratio-type dynamic material-balance concentration controller driven by the integral actions of the primary and secondary loops of the temperature controller and an EKF to recover the concentration. The proposed linear and decentralized approach was tested with a representative case example through numerical simulations in a worst-case situation where the open-loop unstable steady-state coincide with the maximum reaction rate implying lack of local observability, showing a similar and more robust performance with respect the more complex OF passive controller.

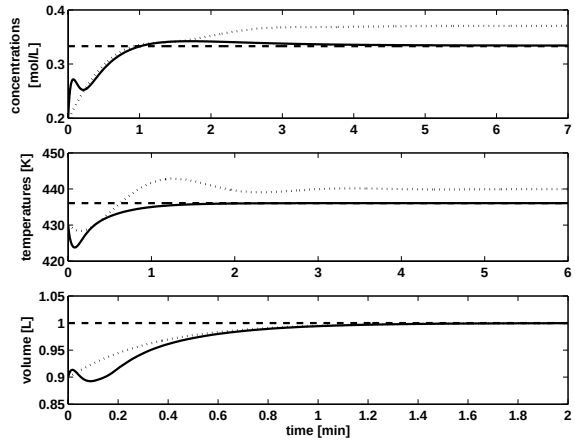

Figure 4. Closed-loop robust behavior with (9,10) nonlinear passivated OF (..) and (22,23,24) PI-inventory OF (-) control.

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