Feedforward-output feedback control for a class of exothermic packed bed tubular reactors

Israel Nájera *, Jesús Álvarez * and Cesar Gutiérrez*

* *Departamento de Ingeniería de Procesos e Hidráulica,*
Universidad Autónoma Metropolitana-Iztapalapa, Apdo. 55534, 09340 México, D.F. México

Abstract: The problem of controlling an open-loop unstable exothermic jacketed packed bed tubular (spatially distributed) reactor through robust feedforward-output feedback (FF-OF) control is addressed. The unmeasured exit concentration must be regulated by adjusting the coolant temperature according to the feed and one interior temperature (in a location to be determined) as well as feed flow measurements. First, the robust nonlinear FF-OF stabilizing control problem is regarded with a staged model, yielding: (i) solvability conditions with a sensor location criterion, and (ii) closed-loop robust stability conditions coupled with simple tuning guidelines. Then, the behavior of this controller is through a simplified model tailored according to passivity and observability properties, yielding an upgraded version of an industrial PI controller, with: antiwindup protection, and feedforward dynamic setpoint compensation. The approach is applied to a representative case example through numerical simulations.

Keywords: Packed bed tubular reactor, spatially distributed system, feedforward control, output-feedback control, passive control, PI control.

1. INTRODUCTION

Spatially distributed fixed packed bed reactors are important units in the chemical and petrochemical industries (Rase, 1990) that exhibit complex nonlinear dynamics with open-loop instability, multiplicity, parametric sensitivity, limit cycling, and structural instability due to close to bifurcation condition (Jensen et al., 1982; Dostal et al., 2009). Basically, these reactors are controlled with temperature PI controllers (Shinskey, 1988; Jaisathaporn et al., 2004; Del Vecchio et al., 2005; Singh et al., 2008). The safety, reactant-to-product yield and selectivity are indirectly ensured and attained by regulating the temperature at a sensitive location by adjusting the heat exchange rate. Even though PI controllers are robust and cheap, their design and supervision rely heavily on per-reactor experience, testing and supervision (Vernieres-Hassimi, 2012). Thus, there is an incentive to systematize and improve existing PI controllers.

These considerations motivate the present study on the development of a more systematic PI control design, including: (i) criterion for sensor location and number, (ii) guarantee of closed-loop robustly stable functioning, (iii) antiwindup protection, and (iv) the possibility of enhancing the disturbance rejection capability through a feedforward (FF) component driven by measured feed temperature and flow disturbances.

In advanced control two approaches are employed: (i) late lumping (the control is designed using the PDE model and is discretized at implementation), and (ii) early lumping (the controller is designed with a discretized model). While the estimation and control theory for nonlinear finite-dimensional systems has advanced significantly in the last two decades (Sepulchre et al., 2011), the theory for nonlinear distributed systems lags behind, and their control design is still an open subject of research (Christofides, 2001; Padhi et al., 2009). Most of the advanced estimation and control studies in chemical tubular reactors have been performed with early lumping approach (Christofides, 2001).

In this study, the problem of designing a feedforward-output feedback (FF-OF) control scheme to regulate the unmeasured exit concentration of an open-loop unstable exothermic packed bed reactor by manipulating the coolant temperature according to one temperature measurement along the reactor is addressed. The aim is to obtain a control scheme, as simple as possible in terms of nonlinearity, coupling, and model dependency, and tuning.

2. CONTROL PROBLEM

Consider the jacketed packed bed tubular reactor, depicted in Fig. 1 with conventional □ (or proposed □+□) control scheme, where a reactant is fed at volumetric flow rate (q), temperature (T_e) and concentration (C_e) and converted into product through an exothermic reaction.

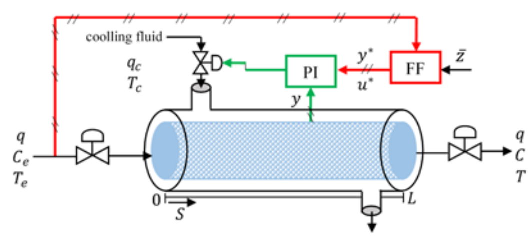

Fig. 1. Tubular reactor and control scheme.

Under standard assumptions (Rase, 1990), the reactor dynamics, in dimensionless form, are given by the PDE's

$$0 = -q\,\partial_s c - r(c,\tau),\ \ 0 \le s \le 1;\ s = 0{:}\ c = c_e \qquad \text{(1a-b)}$$
$$\partial_t \tau = \mathfrak{D}_h\,\partial_{ss}\tau - q\,\partial_s \tau + \beta r(c,\tau) - \delta(\tau - \tau_c), 0 \le s \le 1 \qquad \text{(1c)}$$
$$s = 0{:} \mathfrak{D}_h\,\partial_s \tau = q(\tau - \tau_e); = 1{:}\ \partial_s \tau = 0;\ \ t = 0{:}\ \tau = \tau_0 \qquad \text{(1d-f)}$$
$$z = c(1,t);\ u = \tau_c;\quad y = \tau(s_m, t),\ \ s_m \in M = [0,1] \qquad \text{(1g-h)}$$
$$\boldsymbol{d} = (q, \tau_e)^T; \qquad \text{(1i)}$$

that correspond to the distributed mass and energy balances, where $c(s,t)$ [or $\tau(s,t)$] is the concentration (or temperature) time-varying spatial profile, t is the time, s is the axial length, $\mathfrak{D}_h$ is the heat dispersion number, β is the adiabatic temperature, δ is the heat transfer parameter, and r is the reaction rate. The exit concentration z is the *regulated output*, the temperature y at the axial location s_m (to be determined) is the *measurement for feedback control*, the coolant temperature u is the *manipulated input*, $\boldsymbol{d}$ is the vector of *measured disturbances* made of feed temperature τ_e and flow rate q, and the feed concentration c_e is reasonably constant.

Reactor (1) exhibits the complex nonlinear behavior of an important class of industrial reactors (Eigenberg, 1975; Jensen et al., 1982; Jorgensen, 1986): steady-state multiplicity, parametric sensitivity, structural instability, and hot spot in the temperature profile.

The *problem* consists in designing a feedforward-output feedback (FF-OF) robust stabilizing controller for reactor (1), to indirectly regulate the unmeasured exit concentration z about its prescribed value $\bar{z}$ through the direct regulation of the reactor temperature y, at a suitable location s_m (to be determined), about its corresponding nominal value $\bar{y}$ by manipulating the control input u in spite of the measured disturbance $\boldsymbol{d}$. We are interested in drawing an application-oriented reliable control scheme as simple as possible, in the sense of linearity, dynamical decoupling, and model independence. This rules out the direct implementation of a model-based advanced OF controller.

Without restricting the approach for the reactor class (1), let us consider as representative *case example* an irreversible first-order exothermic reaction $r(c,\tau)$ with Arrhenius temperature dependency (2a) and the parameters (2b-c) (Eigenberg, 1975):

$$r(c,\tau) = c\alpha(\tau), \quad \alpha(\tau) = \exp(\phi - \gamma/\tau) \tag{2a}$$
$$\phi = 21.82, \quad \gamma = 25, \beta = 0.5, \delta = 1, \mathfrak{D}_h = 0.2 \tag{1b}$$
$$\bar{c}_e = \bar{\tau}_e = q = 1, \quad \bar{\tau}_c = 1.0 \tag{2c}$$

The corresponding reactor (1) has the three steady-state (SS) profile pairs $[\bar{c}(s), \bar{\tau}(s)]_{i=1,\ldots 3}$ shown in Fig. 2, with two stable SSs (continuous curves 1, and 3), and one unstable SS (discontinuous curves 2). The reactor *must operate about the unstable* SS $[\bar{c}(s), \bar{\tau}(s)]_2$ with exit concentration $\bar{c}(1) \approx 0.274$ and temperature $\bar{\tau}(1) \approx 1.262$

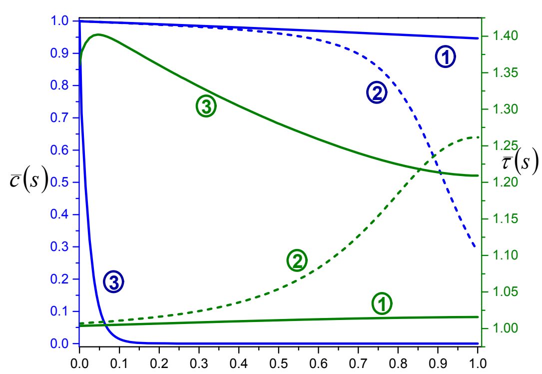

Fig. 2. Steady-state concentration-temperature profiles.

3. FF-SF CONTROL

In this section the model-based nonlinear state-feedback (SF) robust control problem is addressed on the basis of a staged model approximation of the distributed system (1).

3.1 Staged model

In the last decade most of the modeling, estimation and control studies are based on the distributed model (made of partial differential equations -PDEs-) (Christofides, 2001). However, it is known that a staged model (described by ordinary differential equations -ODE's-) can adequately describe the complex tubular reactor dynamics (Deckwer, 1974; Badillo-Hernandez et al., 2013; Nájera et al. 2015).

The application of spatial finite differences to the distributed system (1) yields the N-stage model

$$0 = -\theta\Delta^{-}c_i - r(c_i,\tau_i), \qquad 1 \le i \le N, \qquad z = c_N \tag{3a}$$
$$\dot{\tau}_i = \theta_h\Delta^2\tau_i - \theta\Delta^{-}\tau_i - \delta(\tau_i - u) + \beta r(c_i,\tau_i), \quad y = \tau_m \tag{3b}$$
$$i = 0: \quad c_i = c_e, \qquad \theta_h\Delta^{+}\tau_i = \theta(\tau_i - \tau_e) \tag{3c}$$
$$i = N+1: \qquad \Delta^{-}\tau_i = 0, \quad \boldsymbol{d} = (\theta, \tau_e)^T \tag{3d}$$
$$t = 0: \quad \tau_i(0) = \tau_{i0}; \qquad m \in M = \{1, \ldots, N\} \tag{3e-f}$$

where

$$\theta_m = N^2\mathfrak{D}_m, \theta_h = N^2\mathfrak{D}_h, \theta = Nq, \quad \Delta^{-}(\cdot)_i = (\cdot)_i - (\cdot)_{i-1}$$
$$\Delta^{+}(\cdot)_i = (\cdot)_{i+1} - (\cdot)_i, \quad \Delta^2(\cdot)_i = (\cdot)_{i+1} - 2(\cdot)_i + (\cdot)_{i-1}$$

In compact notation, this model is written as

$$0 = \boldsymbol{\varphi}_c(\boldsymbol{x}_c, \boldsymbol{x}_\tau, u, \boldsymbol{d}), \qquad y = \boldsymbol{c}_y\boldsymbol{x}_\tau \tag{4a}$$
$$\dot{\boldsymbol{x}}_\tau = \boldsymbol{\varphi}_\tau(\boldsymbol{x}_c, \boldsymbol{x}_\tau, u, \boldsymbol{d}), \boldsymbol{x}_\tau(0) = \boldsymbol{x}_{\tau o}, \quad z = \boldsymbol{c}_z\boldsymbol{x}_c \tag{4b}$$
$$\boldsymbol{c}_y\boldsymbol{x}_\tau = \tau_m, \quad \boldsymbol{c}_z\boldsymbol{x}_c = c_N, \quad \dim \boldsymbol{x}_c = \dim \boldsymbol{x}_\tau = N$$

The unique solution for $\boldsymbol{x}_c$ of eq. (4a) followed by substitution in (4b) yields the *N-dimensional staged model*

$$\dot{\boldsymbol{x}}_\tau = \boldsymbol{f}_\tau(\boldsymbol{x}_\tau, u, \boldsymbol{d}), \quad \boldsymbol{x}_\tau(0) = \boldsymbol{x}_{\tau o}, \qquad \dim \boldsymbol{x}_\tau = \boldsymbol{x}_c = N \tag{5a}$$
$$\boldsymbol{x}_c = \boldsymbol{h}_c(\boldsymbol{x}_\tau, u, \boldsymbol{d}), \quad z = h_z(\boldsymbol{x}_\tau, u, \boldsymbol{d}), \quad y = h_y(\boldsymbol{x}_\tau) \tag{5b}$$

where

$$\boldsymbol{x}_c = \boldsymbol{h}_c(\boldsymbol{x}_\tau, u, \boldsymbol{d}) \;\Leftrightarrow \boldsymbol{\varphi}_c(\boldsymbol{x}_c, \boldsymbol{x}_\tau, u, \boldsymbol{d}) = 0 \tag{5c-d}$$
$$\boldsymbol{f}_\tau(\boldsymbol{x}_\tau, u, \boldsymbol{d}) = \boldsymbol{\varphi}_\tau[\boldsymbol{h}_c(\boldsymbol{x}_\tau, u, \boldsymbol{d}), \boldsymbol{x}_\tau, u, \boldsymbol{d}] \tag{5e}$$
$$h_z(\boldsymbol{x}_\tau, u, \boldsymbol{d}) = \boldsymbol{c}_z\boldsymbol{h}_c(\boldsymbol{x}_\tau, u, \boldsymbol{d}), \quad h_y(\boldsymbol{x}_\tau) = \boldsymbol{c}_y\boldsymbol{x}_\tau \tag{5f}$$

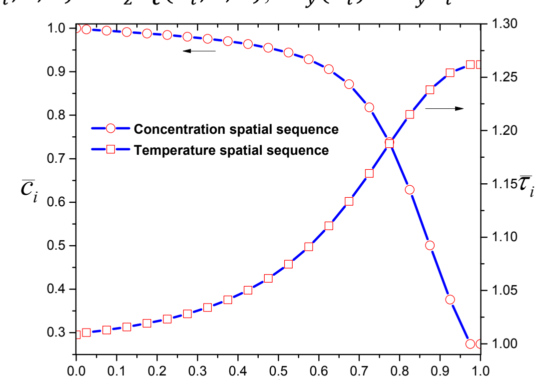

Fig. 3. Staged approximation of the nominal open-loop unstable SS concentration (○) and temperature (□) sequences with $N = 20$ stages, and their interpolated profiles (—).

In Fig. 3 are shown the approximations (up to meaningful transport-kinetics parameter errors) of the nominal SS sequences $[\bar{c}(s), \bar{\tau}(s)]_2$ (# 2 in Fig. 2) with $N = 20$ so that a similar (root mean squared) error with respect to the "almost" distributed approximation (with $N = 100$) is obtained.

3.2 FF concentration regulatory controller

The aim is to keep the effluent concentration z at its nominal value $\bar{z}$ by adjusting control u according to $\boldsymbol{d}$, this is,

$$z(t) = c_N(t) \approx \bar{z} \quad (6)$$

A FF controller is a model-based inverse of the plant (Shinskey,1988) [for given $(\bar{z}, \boldsymbol{d})$ the controller must determine the input u^* so that $z(t) = \bar{z}$], meaning the staged reactor dynamic inverse (Hirschorn, 1979) with respect to its input-output pair (u, z). The dynamic component of the inverse is the z-zero-dynamics (z-ZD) (Isidori, 1989). In industry it is known that the FF-FB scheme is the most effective way to control a difficult process (Shinskey, 1977): the FF executes most of the disturbance rejection, and the FB provides stable output regulation.

The enforcement of the regulation condition (6) yields the dynamic inverse of the staged reactor model (5), or equivalently, the *FF controller*

$$\dot{\boldsymbol{x}}_\tau^* = \boldsymbol{\vartheta}_\tau(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \quad \boldsymbol{x}_\tau^*(0) = \boldsymbol{x}_{\tau o}^*, \quad \dim \boldsymbol{x}_\tau^* = \boldsymbol{x}_c^* = N \quad (7a)$$
$$\boldsymbol{x}_c^* = \boldsymbol{\vartheta}_c(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \quad u^* = \mu^*(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \quad y^* = h_y(\boldsymbol{x}_\tau^*) \quad (7b)$$

where

$$\boldsymbol{\vartheta}_\tau(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}) = \boldsymbol{f}_\tau[\boldsymbol{x}_\tau^*, \mu^*(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \boldsymbol{d}]$$

$$\boldsymbol{\vartheta}_c(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}) = [\eta_{c_1}(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \ldots, \eta_{c_{N-1}}(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \bar{z}]^T$$
$$\eta_{c_i}(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}) = h_{c_i}[\boldsymbol{x}_\tau^*, \mu^*(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \boldsymbol{d}, \bar{z}]$$
$$u = \mu^*(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{\boldsymbol{z}}) \Leftrightarrow h_{c_N}(\boldsymbol{x}_\tau^*, u, \boldsymbol{d}) = \bar{z} \quad (8a\text{-}b)$$

with *z-passive* solvability condition

$$rd(u, z) = 0 \leftrightarrow h_{c_N}(\boldsymbol{x}_\tau, u, \boldsymbol{d}) \; u\text{-monotonic} \quad (9a\text{-}b)$$
$$z\text{-}ZD \text{ (8a) R-stable} \quad (9c)$$

where eq. (9a) denotes the (relative degree-rd- of the input-output pair-u, z) unique solution for u of the algebraic equation (9b), and eq. (9c) states that the associated zero (z-output deviation with respect to $\bar{z}$) dynamics (ZD) must be robustly stable (R-stable).

3.3 FF-SF temperature tracking controller

The task is to track the time-varying setpoint temperature $y^*(t)$ generated by the FF composition controller (7), according to the prescribed dynamics (k is the control gain)

$$\dot{e}_y = -ke_y, \quad e_y = y - y^*(t); \quad (y^*, \dot{y}^*)^T \coloneqq \boldsymbol{\psi} \quad (10a\text{-}b)$$

by manipulating the control u. The enforcement of eq. (10a) on the staged model (5) followed by solution for u yields the *SF temperature tracking controller*

$$u = \mu_y(\boldsymbol{x}_\tau, \boldsymbol{d}, \boldsymbol{\psi}) \Leftrightarrow f_m^\tau(\boldsymbol{x}_\tau, u, \boldsymbol{d}) = \dot{y}^* - k(y - y^*) \quad (11a\text{-}b)$$

Eq. (11a) is the unique solution for u of the algebraic equation (11b). The corresponding inverse dynamics are

$$\dot{\boldsymbol{x}}_\zeta^* = \boldsymbol{f}_\tau^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \boldsymbol{\psi}), \quad \boldsymbol{x}_\zeta^*(0) = \boldsymbol{x}_{\zeta o}^*, \quad \dim \boldsymbol{x}_\zeta^* = N - 1 \quad (12a)$$
$$\boldsymbol{x}_c^* = \boldsymbol{h}_c^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \boldsymbol{\psi}); \quad z^* = h_z^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \boldsymbol{\psi}); \quad y = y^* \quad (12b\text{-}d)$$
$$u = \mu_y(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \boldsymbol{\psi}); \quad \boldsymbol{x}_\tau^* = \boldsymbol{I}_m(\boldsymbol{x}_\zeta^{*T}, y^*)^T \quad (12e\text{-}f)$$

where

$$\boldsymbol{f}_\tau^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \boldsymbol{\psi}) = \boldsymbol{f}_\tau[\boldsymbol{x}_\zeta^*, \mu_y(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \boldsymbol{\psi}), \boldsymbol{d}]$$
$$\boldsymbol{h}_c^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \boldsymbol{\psi}) = \boldsymbol{h}_c[\boldsymbol{x}_\zeta^*, \mu_y(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \boldsymbol{\psi}), \boldsymbol{d}]$$
$$h_z^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \boldsymbol{\psi}) = h_z[\boldsymbol{x}_\zeta^*, \mu_y(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \boldsymbol{\psi}), \boldsymbol{d}]$$

The related y-*passivity* (Isidori, 1989) solvability condition is

$$rd(u, y) = 1 \leftrightarrow f_m^\tau(\boldsymbol{x}_\tau, u, \boldsymbol{d}) \; u\text{-invertible} \quad (13a\text{-}b)$$
$$y\text{-}ZD \text{ (12) R-stable}, m \in M \quad (13c)$$

Eq. (13a) states that the staged reactor model (5) is passive with relative degree equal to one with respect to the input-output pair (u, y) (with measurement y at stage m), and Eq. (13b) that the motions $\boldsymbol{x}_\tau^*(t)$ of the associated $(N-1)$-dimensional nonautonomous y-ZD (12) are robustly stable.

3.4 Cascade FF-SF dynamic nonlinear controller

Assuming for the moment that the temperature state sequence $\boldsymbol{x}_\tau$ is known, the combination of the FF composition regulatory (7) and temperature tracking (11) controllers yields the *composition-temperature cascade controller*

$$\dot{\boldsymbol{x}}_\tau^* = \boldsymbol{\vartheta}_\tau(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}), \qquad \boldsymbol{x}_\tau^*(0) = \boldsymbol{x}_{\tau o}^* \quad (14a)$$
$$\boldsymbol{\psi} = \boldsymbol{\vartheta}_\psi(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z}); \qquad u = \mu_y(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \boldsymbol{\psi}) \quad (14b\text{-}c)$$
$$\boldsymbol{\vartheta}_\psi(\boldsymbol{x}_\tau^*, \boldsymbol{d}) = \left[h_y(\boldsymbol{x}_\tau^*), \vartheta_m^\tau(\boldsymbol{x}_\tau^*, \boldsymbol{d}, \bar{z})\right]^T$$

with z-pasivity (9) and y-passivity (13) conditions

4. REDESIGNED FF-SF CONTROL

In this section the solvability of the FF-FB cascade controller (14) is assessed, finding that the primary control is not stable. Then the control scheme is redesigned accordingly.

4.1 Solvability

In terms of rd conditions with physical meaning, the solvability conditions (16) of the cascade control (15) are

$$rd(u, z) = 0 \leftrightarrow \delta, \theta \neq 0, \quad z\text{-}ZD \text{ (8a) R-stable} \quad (15a\text{-}b)$$
$$rd(u, z) = 1 \leftrightarrow \delta \neq 0, \quad y\text{-}ZD\text{(13a) R-stable } m \in M \quad (15c\text{-}d)$$

Eqs. (15a) an (15c) are robustly met because the heat exchange coefficient ($\delta > 0$) and dilution rate ($\theta > 0$) are sufficiently strictly positive.

The sensor location can be established by looking at: (i) the largest absolute value of the dominant eigensequence of the linearization of the y-ZD (Nájera et al., 2015), (ii) the largest absolute value of the temperature (discrete) gradient $\Delta^- \tau_i$ (zero concavity criterion $\Delta^2 \tau_i \approx 0$) (Bashir et al. 1992; Porru et al., 2014; Nájera et al., 2015). Here, first the concavity criterion will be used to obtain a suggestive results, and then the location will be tuned (in section 7) against control functioning in order to draw the best location with respect to closed-loop behavior.

Accordingly, in Figure 4 are plotted the temperature as well as the temperature gradient and concavity spatial sequences associated to the open-loop unstable reactor, yielding that, in order to obtain a R-stable y-ZD the sensor must be located at stage 14 or 15, this is,

$$m = 14 \; or \; 15 \quad \Rightarrow \quad s_m \in [0.68, \; 0.73] \quad (16a\text{-}b)$$

meaning that the sensor should be in the middle of the dimensionless interval $[0.68, 0.73]$ of the actual reactor.

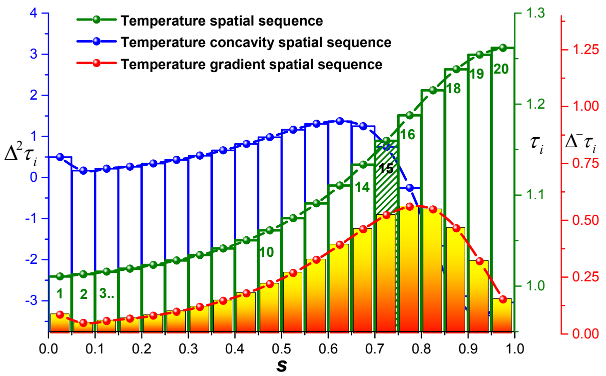

Fig 4. Temperature as well as temperature gradient and concavity spatial sequences of the open-loop unstable staged reactor.

Comparing with our previous stage interval for a tubular reactor (with concentration-dynamic coupling, R-stable y-ZD at the stage interval 1-to-13, and smallest concavity at stage 8), here the stage interval for y-ZD R-stability is just 14-15. This is so because, in spite of the lack of concentration dynamics, the present packed bed gas reactor has a more complex nonlinear behavior.

Summarizing, as it stands the FF-SF cascade controller cannot be implemented because its FF composition component is unstable.

4.2 Redesigned FF-SF cascade controller

Following the approach employed in previous distillation (Porru et al., 2014) and tubular reactor (Nájera et al., 2015) studies, here the primary component (14a) of the cascaded controller (14) is redesigned in to obtain a R-stabilizing FF-SF controller.

Rewrite the primary controller (7a) as follows

$$\dot{\boldsymbol{x}}_\tau^* = \boldsymbol{f}_\tau(\boldsymbol{x}_\tau^*, u^*, \boldsymbol{d}) \;\; \boldsymbol{x}_\tau^*(0) = \boldsymbol{x}_{\tau o}^*; \quad u^* = \mu^*(\boldsymbol{x}_\tau, \boldsymbol{d}, \bar{\boldsymbol{z}}) \quad \text{(17a-b)}$$

omit the state accumulation ($\dot{\boldsymbol{x}}_\tau^* = 0$), replace $(\boldsymbol{x}_\tau^*, u^*)$ in (17a) by $(\boldsymbol{x}_\tau^{\mathrm{s}}, u_s)$,

$$\boldsymbol{f}_\tau(\boldsymbol{x}_\tau^{\mathrm{s}}, u_s, \boldsymbol{d}) = 0;\;\; u_s = \mu^*(\boldsymbol{x}_\tau^{\mathrm{s}}, \boldsymbol{d}, \bar{z});\;\; (\boldsymbol{x}_\tau^{\mathrm{s}}, u_s) \neq (\boldsymbol{x}_\tau^*, u^*) \quad \text{(18a-c)}$$

For given $(\boldsymbol{d}, \bar{z})$, The solution for the N-variable set $(\boldsymbol{x}_\tau^{\mathrm{s}}, u_s)$ of the last N-algebraic equations set is denoted by:

$$\boldsymbol{x}_s = (\boldsymbol{x}_\tau^{sT}, u_s)^T = \boldsymbol{\sigma}(\boldsymbol{d}, \bar{z}) \;\leftrightarrow\; \boldsymbol{x}_\tau^{\mathrm{s}} = \boldsymbol{\sigma}_\tau(\boldsymbol{d}, \bar{z}),\, u_s = \sigma_u(\boldsymbol{d}, \bar{z})$$

and the m-th element of $\boldsymbol{\sigma}_\tau(\boldsymbol{d}, \bar{z})$ yields the dependency of the static assumption-based temperature setpoint on the measured-given data $(\boldsymbol{d}, \bar{z})$, according to the expression

$$y_s = \sigma_{\tau_m}(\boldsymbol{d}, \bar{z}) \coloneqq \rho(\boldsymbol{d}, \bar{z}) \quad \text{(19)}$$

To compensate for the omission of the accumulation term ($\dot{\boldsymbol{x}}_\tau^* = 0$ in eq. 17a) in the calculation of the preceding static setpoint approximation (19), let us add a first order lag (20a) to (19) in order to get the dynamic stable the *setpoint compensator* (with gain $k_* \approx \lambda_y$)

$$\dot{y}^* = -k_*(y^* - y_s),\;\; y^*(0) = y_0^*;\;\; y_s = \rho(\boldsymbol{d}, \bar{z}) \quad \text{(20a-b)}$$

where λ_y is the characteristic time of the open-loop temperature response. The related solvability condition

$$\det \boldsymbol{J}(\boldsymbol{x}_\tau^{\mathrm{s}}, \boldsymbol{d}, u_s) \neq 0,\quad \boldsymbol{J}(\boldsymbol{x}_\tau^{\mathrm{s}}, \boldsymbol{d}, u_s) = \partial_{\boldsymbol{x}_s}\boldsymbol{f}_s(\boldsymbol{x}_s, \boldsymbol{d}, \bar{z}) \quad \text{(21)}$$

$$\boldsymbol{f}_s(\boldsymbol{x}_s, \boldsymbol{d}, \bar{z}) = [\boldsymbol{f}_\tau^T(\boldsymbol{x}_\tau^{\mathrm{s}}, u_s, \boldsymbol{d}), \mu^*(\boldsymbol{x}_\tau^{\mathrm{s}}, \boldsymbol{d}, \bar{z}) - u_s]^T$$

is the z-passivity, with $rd = 0$ (Khalil, 2002) for $(\bar{z}, y_s)$, of the static component (20b). Since the dynamic component (20a) is passive, with $rd = 1$ for (y_s, y^*), the setpoint compensator (20) is passive with respect to $(\bar{z}, y^*)$.

Recall the inverse dynamics-based cascade controller (14) and replace its unstable FF component (14a) with is stable approximation (20) to obtain the *stable dynamic cascade controller*

$$\dot{y}^* = -k_*(y^* - y_s),\;\; y^*(0) = y_0^*;\quad y_s = \rho(\boldsymbol{d}, \bar{z}) \quad \text{(22a-b)}$$
$$u = \mu(\boldsymbol{x}_\tau, \boldsymbol{d}, u, y^*, y_s) \quad \text{(22c)}$$

where μ denotes the unique solution for u of the equation

$$f_m^\tau(\boldsymbol{x}_\tau, u, \boldsymbol{d}) = -k_*(y^* - y_s) - k_y(y - y^*)$$

The corresponding solvability condition (15) become

$$det\, J(\boldsymbol{x}_\tau^{\mathrm{s}}, \boldsymbol{d}, u_s) \neq 0,\;\; \theta \neq 0,\;\; \delta \neq 0,\;\; m \in M \quad \text{(23a-d)}$$

5. FF-OF CONTROL

The combination of the passivated cascade controller (22) with a geometric observer, with robust second-order detectability innovation structure (Fernandez et al., 2012), yields the *robust FF-OF controller*

$$\dot{y}^* = -k_*(y^* - y_s),\;\; y^*(0) = y_0^*;\quad y_s = \rho(\boldsymbol{d}, \bar{z}) \quad \text{(24a-b)}$$
$$\dot{\hat{\boldsymbol{x}}}_\tau = \boldsymbol{f}_\tau(\hat{\boldsymbol{x}}_\tau, u, \boldsymbol{d}) + \boldsymbol{g}_y(\hat{\boldsymbol{x}}_\tau, u, \boldsymbol{d})(y - \boldsymbol{c}_y\hat{\boldsymbol{x}}_\tau) \quad \text{(24c)}$$
$$+\, \boldsymbol{g}_\iota(\hat{\boldsymbol{x}}_\tau, u, \boldsymbol{d})\hat{\iota};\;\; \hat{\boldsymbol{x}}_\tau(0) = \hat{\boldsymbol{x}}_{\tau_o}$$
$$\dot{\hat{\iota}} = \omega_y^3(y - \boldsymbol{c}_y\hat{\boldsymbol{x}}_\tau),\qquad \hat{\iota}(0) = \hat{\iota}_o \quad \text{(24d)}$$
$$u = \mu(\hat{\boldsymbol{x}}_\tau, u, \boldsymbol{d}, y^*, y_s) \quad \text{(24e)}$$

where $dim(y^*, \hat{\boldsymbol{x}}', \hat{\iota})^T = N + 2 = 22$,

$$\boldsymbol{g}_i(\boldsymbol{x}_\tau, \boldsymbol{d}, u) = [\boldsymbol{0}^{\boldsymbol{T}}, \boldsymbol{O}^{-1T}(\boldsymbol{x}_\tau, \boldsymbol{d}, u)\boldsymbol{k}_i, \boldsymbol{0}^T]^T,\quad i = y, \iota$$
$$\boldsymbol{O}(\boldsymbol{x}_\tau, \boldsymbol{d}, u) = \partial_{\boldsymbol{x}_\iota}\boldsymbol{\varpi}(\boldsymbol{x}_\tau, \boldsymbol{d}, u)$$
$$\boldsymbol{\varpi}(\boldsymbol{x}_\tau, \boldsymbol{d}, u) = [\tau_m, f_m^\tau(\boldsymbol{x}_\tau, \boldsymbol{d}, u)]^T$$
$$\boldsymbol{k}_y = (2\zeta_y + 1)(\omega_y, \omega_y^2)^T,\, \boldsymbol{k}_\iota = (0,1)^T, \zeta_y[1,3], \omega_y \in [5,10]\lambda_y$$

$\boldsymbol{g}_y$ (or $\boldsymbol{g}_\iota$) is the proportional (or integral) nonlinear gain, ζ_y (or ω_y) is the damping factor (or characteristic frequency) of the output convergence dynamics. The related generic solvability conditions are:

$$det\, J(\boldsymbol{x}_\tau^{\mathrm{s}}, \boldsymbol{d}, u_s) \neq 0;\quad \theta, \delta, \beta \neq 0;\quad m \in M \quad \text{(25a-c)}$$

which in our case become (25) with m = 14 or 15 (16). The sensor location criteria (23c) for the secondary control (24e) coincides with the one for state estimation (24c-d) (Fernandez et al., 2012). This agrees with previous studies and industrial practice (Harris et al., 1980).

However, the dynamic FF-OF controller (24) is too complex in comparison to its PI industrial counterparts (Jaisathaporn et al., 2004; Del Vecchio et al., 2005), in the sense of: (i) highly nonlinear interaction, (ii) $N + 2$ ODEs (22 for our case example) must be on-line integrated. The overcoming of this applicability obstacle is the subject of the next section.

6. SIMPLIFIED FF-OF CONTROLLER

In this section, the functioning staged model-based robust FF-OF controller (24) is recovered with a simplified controller built according to passivity and observability.

6.1 Secondary controller redesign

Let us recall the N-stage model (5) and express its y-output dynamics in the form (Gonzalez and Alvarez, 2005)

$$\dot{y} = au + \iota; \quad \iota = f_m^\tau(\boldsymbol{x}_\tau, \boldsymbol{d}, u) + au, \quad a \approx \bar{a} \tag{26a-b}$$
$$rd(u, y) = rd(\iota, y) = 1, \quad \bar{a} = (\partial_u f_m^\tau)(\bar{\boldsymbol{x}}_\tau, \bar{\boldsymbol{d}}, \bar{u}) > 0$$

$f_{\tau m}$ is defined after (11), ι is an observable input, and (u, ι) satisfies the matching condition (Sepulchre, 2011). The elimination of the static nonlinear component (26b) in eq. (26) yields the *simplified model*

$$\dot{y} = au + \iota, \qquad rd(u, y) = rd(\iota, y) = 1 \tag{27a-b}$$

for temperature control design, with unmeasured-observable input ι. The enforcement of the tracking condition (10a) upon this model yields the controller (11) in the ι-dependent form (28a), and a convergent estimate $\hat{\iota}$ of input ι of model (27a) is given by the reduced-order observer (28b) with adjustable (up to measurement noise) exponential convergence rate ω (Gonzalez and Alvarez, 2005):

$$u = [k_*(y^* - y_s) + k(y - y^*) + \iota]/a \tag{28a}$$
$$\dot{\chi} = -\omega\chi - \omega(\omega y - au), \quad \chi(0) = 0, \quad \hat{\iota} = \chi + \omega y \tag{28b}$$

The combination of control (28a) (with $\iota = \hat{\iota}$) with observer (28b) yields the dynamic *temperature tracking controller*

$$\dot{\chi} = -\omega\chi - \omega(\omega y + au), \qquad \chi(0) = 0 \tag{29a}$$
$$u = [k_*(y^* - y_s) + \omega y^* + (k + \omega)(y - y^*) + \chi]/a \tag{29b}$$

with one linear ODE, and similar behavior than the one (24c-e) of its detailed model-based counterpart (24). This control has antiwindup protection because the χ-dynamics (29a) runs regardless of control saturation (Díaz-Salgado et al., 2012).

6.2 PI temperature controller with FF setpoint compensation

The combination of the primary (22a-b) and redesigned secondary (29) control yields the *simplified FF-OF control*:

$$\dot{y}^* = -k_*(y^* - y_s), \quad y_s = \rho(\boldsymbol{d}, \bar{z})(\boldsymbol{d}\text{-feedforward}) \tag{30a-b}$$
$$\dot{\chi} = -\omega\chi - \omega(\omega y - au), \quad \chi(0) = 0 \ (y\text{-feedback}) \tag{30c}$$
$$u = [k_*(y^* - y_s) + \omega y^* + (k + \omega)(y - y^*) + \chi]/a \tag{30d}$$

with: (i) two linear ODEs, and (ii) and similar behavior than the one of its detailed model-based counterpart (24) with $N + 2$ ODEs (22 for case example).

For applicability and comparison purposes, assume there is no saturation and express controller (30) in PI form

$$\dot{y}^* = -k_*(y^* - y_s), \ y^*(0) = y_0^*; \qquad y_s = \rho(\boldsymbol{d}, \bar{z}) \tag{31a-b}$$
$$u_f = \bar{u} + k_*(y^* - y_s), \qquad u = u_f + \pi(y - y^*) \tag{31c}$$

where

$$\pi(e) = \kappa[e + t^{-1} \textstyle\int_0^t e \, dt], \ e = y - y^*, \ \kappa = k/a, \ t = 1/\omega$$

and κ (or t) is the proportional gain (or reset time). This signifies that the proposed controller (30) is an upgraded version the conventional PI:

$$u = \bar{u} + \pi(y - y^*) \tag{32}$$

temperature control employed in industrial reactors (Del Vecchio et al., 2005), with the upgrade consisting in: (i) conventional-like tuning guidelines coupled with closed-loop robust stability assessment, (ii) antiwindup protection, and (iii) load measurement-based FF dynamic setpoint compensation.

7. CONTROL IMPLEMENTATION

The FF-OF controller (30) is tested and compared with its conventional counterpart (32) (with fixed set-point), for the case example (2) with $N = 20$, open-loop instability, and sensor at $m = 15$. The objective is to stabilize the open-loop unstable SS $[\bar{c}(s), \bar{\tau}(s)]_2$ (Fig. 2) with regulation of the exit concentration $z \approx \bar{z} = 0.274$ in spite of large feed temperature step disturbances.

The function $\rho(\boldsymbol{d}, \bar{z})$ of the static FF component (30b) can be written as $\zeta(d_s)$ (33a) and (rather well) approximated by the regression-based curve $\hat{\zeta}(d_s)$, according to the expressions

$$y_s = \rho(\boldsymbol{d}, \bar{z}) = \zeta(d_s) \approx \hat{\zeta}(d_s), \quad d_s = \theta\tau_e \tag{33a}$$
$$\hat{\zeta}(d_s) = a_2 + a_2 d_s + a_3 d_s^2 + a_4 d_s^3 \tag{33b}$$
$$a_1 = -7.8\text{x}10^3, \quad a_2 = 3.70, \quad a_3 = -4.14, \quad a_4 = 1.6$$

The corresponding plot is presented in Figure 5.

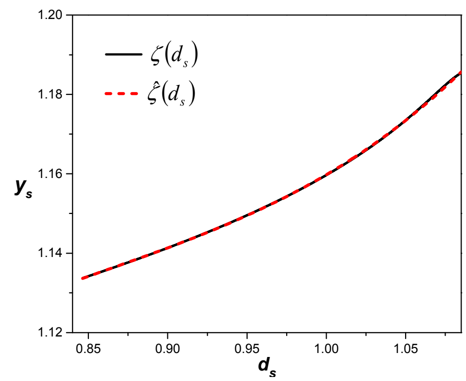

Fig.5. Static element $y_s = \zeta(d_s) \approx \hat{\zeta}(d_s)$ (33) of the setpoint compensator: $\zeta(d_s)$ with $N = 20$ (—), and $\hat{\zeta}(d_s)$ (---).

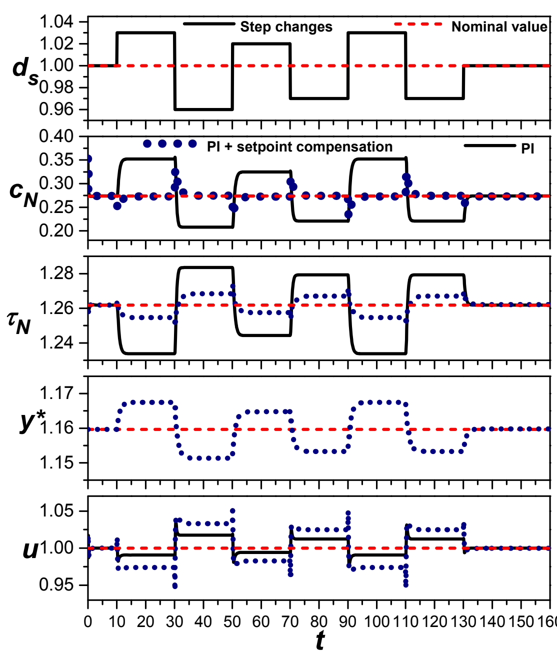

Fig.6 Closed-loop behavior with PI temperature control and feed temperature step disturbances, with (••) and without (—) setpoint compensation.

The application of conventional-like tuning guidelines (Gonzalez and Alvarez, 2005) with simulated measurement noise yielded (after a few iterations) the following gains for control (26) ($\lambda_y \approx q_r \approx 0.875$: open-loop characteristic time)

$$k_* = \lambda_y, \quad k = n_y\lambda_y, \quad \omega = n_\omega k, \quad n_y = 2.6, \quad n_\omega = 5$$

In Fig. 6 are presented the behaviors of the standard (with fixed setpoint) (32) and proposed (with setpoint compensation) (31) controllers when the reactor is subjected to a sequence of dilution rate (θ) and feed temperature (τ_e) step changes, showing that the proposed controller (31): (i) robustly stabilizes the reactor, and (ii) in comparison to its standard PI counterpart (32), reduces by $\approx 86\%$ the variability bound of the exit concentration.

7. CONCLUSIONS

The problem of regulating with robust closed-loop stability the exit concentration of an open-loop unstable packed bed tubular reactor (in spite of feed temperature and flow disturbances) has been resolved designing an OF controller with dynamic setpoint compensation. The dynamic setpoint compensation was driven in FF manner by the measured load disturbances, this compensator had a precomputed N-stage model-based nonlinear static component with an on-line linear first-order lag. Advanced control theory was applied: (i) to develop an N-stage model-based FF-OF robust stabilizing controller with a large number ($N + 2$) of nonlinear ODEs, and (ii) then, to approximate its behavior with a considerably simpler application-oriented controller with only two linear ODEs. The simple controller amounted to an upgrade (dynamic setpoint compensation, simple tuning guidelines, and antiwindup protection) of the standard PI temperature controller employed in industrial practice.

REFERENCES

Badillo-Hernandez, U., Alvarez-Icaza, L., & Alvarez, J. (2013). Model design of a class of moving-bed tubular gasification reactors. *Chem. Eng. Sci.*, 101, 674-685.

Bashir, S., Chovln, T., Masri, B. J., Mukherjee A., Pant A., Sen S., and Vijayaraghavan P., (1992). Thermal Runaway Limit of Tubular Reactors, Defined at the Inflection Point of the Temperature Profile. *Ind. Eng. Chem. Res.*, 31, 2164-2171.

Christofides, P. D. (2001). *Nonlinear and robust control of PDE systems: Methods and applications to transport-reaction processes.* Birkhäuser, Boston.

Deckwer, W., (1974). The Backflow Cell Model-Applied to Non-isothermal Reactors, *The Chemical Engineering Journal*, 8, 135-144.

Del Vecchio, E., Petit, N., (2005). Boundary control for an industrial under-actuated tubular chemical reactor, *Journal of Process Control*, 15, 771-784.

Díaz-Salgado, J., Alvarez, J., Schaum, A., Moreno, J. A. (2012). Feedforward output-feedback control for continuous exothermic reactors with isotonic kinetics. Journal of Process Control, 22(1), 303-320.

Dostál P., Bobál V., and Vojtěšek J. (2009). Adaptive Temperature Control in a Tubular Chemical Reactor, *17th Mediterranean Conference on Control & Automation*, 1209-1214.

Eigenberg, G. (1975), Influence of the Wall on the Dynamic Behavior of Homogeneous Tubular Reactors with a Highly Exothermic Reaction, Chemical Reaction Enginng-II Ch3, *Advances in chemistry series*, 133, 477-488.

Fernandez, C., Alvarez, J., Baratti, R., and Frau, A. (2012). Estimation structure design for staged systems. *Journal of Process Control*, 22 (10), 2038-2056.

Gonzalez, P. and Alvarez, J. (2005). Combined Proportional/Integral-Inventory Control of Solution Homopolymerization Reactors. *Ind. Eng. Chem. Res.*, 44, 7147-7163.

Harris, T. J., Macgregor, J. F., and Wright J. D., (1980) Optimal sensor location with an application to a packed bed tubular reactor. *AIChE Journal*, 26 (6), 910-916.

Hirschorn, R. M. (1979). Invertibility of Nonlinear Control Systems. SIAM *Journal of Control and Optimization*. 17 (2), 289-297.

Isidori, A. (1989). *Nonlinear Control Systems*, Springer-Verlag, Berlin.

Jaisathaporn, P.,Luyben, W. L. (2004). Dynamic Comparison of Alternative Tubular Reactor Systems. *Ind. Eng. Chem. Res.*,43 (4), 1003-1029.

Jensen, K. F., and Ray, H. W. (1982). The bifurcation behavior of tubular reactors. *Chem. Eng. Sci.*, 37 (2), 199-22.

Jorgensen, S. B. (1986). Fixed bed reactor dynamics and control-a review, *Proc. IFAC Control of Distillation Columns and Chemical Reactors*, 11-24.

Khalil H. K. (2002). *Nonlinear systems,* Prentice Hall, NJ

Nájera, I. Álvarez, J., Baratti, R. (2015). Feedforward output-feedback for a class of exothermic tubular reactors, *Proceedings of the 9th ADCHEM.*

Padhi R., Ali S. F., (2009). An account of chronological developments in control of distributed parameter systems, *Annual Reviews in Control*, 33, 59-68.

Porru, M., R. Baratti, J. Alvarez, (2014). Feedforward-feedback control of an industrial multicomponent distillation column, *Proceedings of the 19th IFAC WC*, 19 (Part 1), 1266-1271.

Rase, H. F., (1990). *Fixed-bed reactor design and diagnostics: gas-phase reactions*, Butterworth Publishers, USA.

Sepulchre, R., Jankovic, M., Kokotovic, P.V., (2011). *Constructive Nonlinear Control*, Springer, London,

Shinskey, F. G. (1977). *Distillation Control for Productivity and Energy Conservation*, Mc GrawHill New York.

Shinskey, F. G. (1988). *Process Control Systems-Application, Design, and Tuning*. 3rd Ed. McGraw-Hill.

Singh S., Lal S., and Kaistha, N. (2008). Case Study on Tubular Reactor Hot-Spot Temperature Control for Throughput Maximization. *Ind. Eng. Chem. Res.*, 47 (19), 7257-7263.

Vernieres-Hassimi L., Abdelghani-Idrissiy A., Seguin D., Mouhab N. (2012). Unsteady state maximun temperature estimation and localization in a tubular chemical reactor, *International Journal of Chemical Reactor Engineering*, Vol. 10, A78.