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Feedforward ouput-feedback control for a class of exothermic tubular reactors

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Abstract: The problem of regulating the effluent concentration in an open-loop unstable exothermic jacketed reactor is addressed. The coolant temperature must be adjusted according to temperature as well as flow measurements. First, the robust nonlinear feedforward-output feedback stabilizing control problem is addressed with advanced control theory, yielding: (i) solvability conditions with sensor location criterion, and (ii) closed-loop robust stability coupled with simple tuning guidelines. Then, the behavior of the advanced controller is recovered with a PI temperature controller equiped with: (i) antiwindup protection, and (ii) feedforward dynamic setpoint compensation driven by measured (feed temperature and volumetric flow rate) disturbances. The approach is applied to a representative case example through numerical simulations.

Keywords: Tubular reactor, feedforward control, output-feedback control, passive control, PI control.

1. INTRODUCTION

An important class of products are manufactured in tubular exothermic tubular reactors. These reactors are spatially distributed nonlinear dynamical systems (modeled by partial differential equations -PDEs-) which in many cases exhibit complex dynamics: strong parametric sensitivity, multiplicity, limit cycling, and structural instability (Jensen et al., 1982). Due to bifurcation, an open-loop stable reactor may become unstable with input and kinetics-transport disturbances. The control task is the regulation of yield and selectivity with guarantee of robust closed-loop stability.

By far, industrial reactors are controlled with conventional temperature PI controllers (Shinskey, 1988; Jaisathaporn et al., 2004; Singh et al., 2008). Even though these controllers are robust and cheap, their design and supervision rely heavily on per-reactor experience, testing and supervision. Thus, there is an incentive to systematize and improve through upgrade the existing designs. In principle, advanced control theory should contribute in such endeavour.

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 far behind. The control design of nonlinear distributed systems is still an open subject of research (Christofides, 2001; Hoo et al., 2001). The majority of the advanced estimation and control studies in chemical tubular reactors have been performed with early lumping approach: first, the distributed system is discretized with orthogonal collocation or finite element method; then, advanced finite-dimensional control-observer techniques are applied.

These consideration motivate the methodology of the present study: an interlaced control-observer design for the distributed reactor on the basis of finite-dimensional of the reactor control. To concentrate on the fundamental interplay between advanced and conventional control, a rather simple single concentration-temperature pseudo-homogeneous exothermic reactor class will be regarded as case study (Varma et al., 1973). In spite of its simplicity, the reactor example exhibits the complex nonlinear behavior of an important class of industrial reactors (Eigenberg, 1975; Van Heerden, 1958): steady-state multiplicity, parametric sensitivity, structural instability, and hot spot in the temperature profile.

In this study, the problem of designing a feedforward-output feedback (FF-OF) control scheme to regulate (with quick response and reduced offset) the exit concentration of an open-loop unstable exothermic reactor by manipulating the coolant temperature according to reactor temperature and feed flow temperature disturbance measurements is addressed. The aim is to obtain a control scheme, as simple as possible in terms of nonlinearity, coupling, and model dependency, and tuning. We are interested in: (i) ensuring robust closed-loop stability, (ii) identifying the solvability conditions, and (iii) connecting the advanced and conventional control approaches.

2. CONTROL PROBLEM

Consider the jacketed tubular reactor (Fig. 1), 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. The mass and energy balances in dimensionless form are given by the partial differential equations with initial (1e) and boundary (1c,d) conditions, *regulated output* (exit concentration) (z), *measured output* (y), control input (coolant temperature) (u), and *load disturbance inputs* (feed temperature and volumetric flowrate) $(\boldsymbol{d}_e)$:

$$\partial_t c = \mathfrak{D}_m\,\partial_{ss}c - q\,\partial_s c - r(c,\tau),\ t>0,\ 0<s<1 \quad (1a)$$
$$\partial_t \tau = \mathfrak{D}_h\,\partial_{ss}\tau - q\,\partial_s \tau + \beta r(c,\tau) - \delta(\tau-\tau_c) \quad (1b)$$
$$s=0{:}\ \mathfrak{D}_m\,\partial_s c = q(c-c_e),\ \mathfrak{D}_h\,\partial_s \tau = q(\tau-\tau_e) \quad (1c)$$
$$s=1{:}\ \partial_s c = \partial_s \tau = 0;\ t=0{:}\ c=c_0,\ \tau=\tau_0 \quad (1d,e)$$
$$z=c(1,t),\ \ u=\tau_c,\ \ y=\tau(s_m,t),\ \ \boldsymbol{d}_e(t)=(\tau_e,q)' \quad (1f)$$

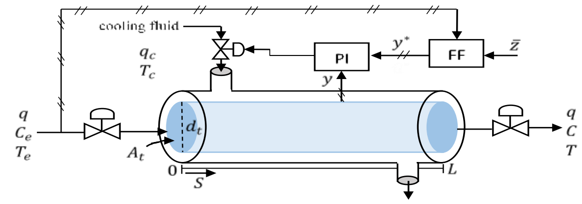

Fig. 1. Tubular reactor and control scheme.

$c(s,t)$ [or $\tau(s,t)$] is the time-varying concentration (or temperature) profile, c_e (or τ_e) is the feed concentration (or temperature), q is the dilution rate, τ_c is the coolant temperature, $\mathfrak{D}_m$ (or $\mathfrak{D}_h$) is the mass (or heat) dispersion number, β is the adiabatic temperature, δ is the heat transfer parameter, and r is the reaction rate. The feed concentration c_e is constant. With suitable modifications (concentration in quasi-steady state, no mass dispersion, packed bed, multicomponent) reactor (1) can be adapted to a diversity of industrial tubular reactors.

The *problem* consists in designing a feedforward (FF)-output-feedback (OF) robust stabilizing controller for an open-loop unstable exothermic tubular reactor. The exit concentration z must be regulated about a prescribed value $\bar{z}$ in spite of feed flow rate and temperature disturbances ($\boldsymbol{d}_e$), by manipulating the control input u (coolant temperature τ_c) according to the two-load input $\boldsymbol{d}_e$ and output (y) (temperature at length s_m) measurements. We are interested in drawing an application-oriented reliable control scheme as simple (linear and dynamically decoupled) and model independent as possible.

Let us recall as case example an extensively studied system (Varma et al., 1973): an irreversible first-order exothermic reaction $r(c,\tau)$ with Arrhenius temperature dependency

$$r(c,\tau)=c\alpha(\tau),\ \alpha(\tau)=\exp(\phi-\gamma/\tau),\ \phi=22.2 \quad (2a)$$
$$\gamma=25,\ \beta=0.5,\ \delta=1,\ \mathfrak{D}_m=\mathfrak{D}_h=0.2$$
$$c_e=\bar{\tau}_e=\bar{\tau}_c=q=1$$

The reactor (1) has the five steady-state (SS) profile pairs $[\bar{c}(s),\bar{\tau}(s)]_{i=1,\dots 5}$ shown in Fig. 2, with three stable SSs (continuous curves 1, 3 and 5), and two unstable SSs (discontinuous curves 2 and 4). The reactor must operate about the unstable SS $[\bar{c}(s),\bar{\tau}(s)]_4$ with: (i) exit concentration $\bar{z}\approx 0.006$, and (ii) temperature hotspot at axial length $s_m \approx 0.47$.

3. STAGED MODEL-BASED FEEDFORWARD STATE-FEEDBACK (FF-SF) ROBUST CONTROL

Here the model-based nonlinear feedforward state-feedback (FF-SF) robust control problem is addressed on the basis of a staged model approximation of the distributed system (1). The purposes are: (i) the identification of the solvability conditions, and (ii) the setting of the constructive point of departure for the development (in sections 4 to 6) of an application-oriented FF-OF control scheme.

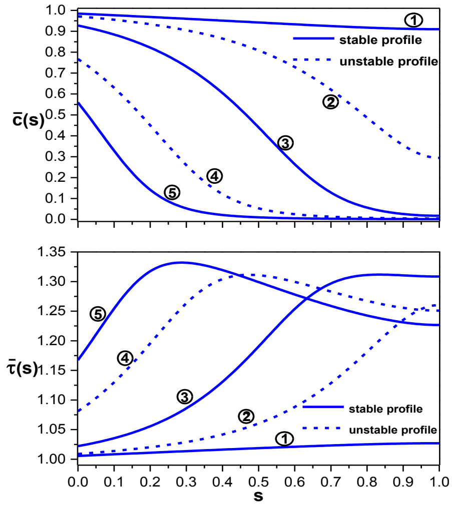

Fig. 2. Steady-state concentration-temperature profiles.

3.1 Staged model

The application of spatial finite differences (over N domain nodes and two boundary ones) to the distributed system (1) yields the n-dimensional model

$$\dot{c}_i=\theta_m\Delta^2 c_i-\theta\Delta^- c_i - r(c_i,\tau_i),\ 1\le i\le N,\qquad z=c_N \quad (3a)$$
$$\dot{\tau}_i=\theta_h\Delta^2\tau_i-\theta\Delta^-\tau_i-\delta(\tau_i-u)+\beta r(c_i,\tau_i),\quad y=\tau_m \quad (3b)$$
$$i=0{:}\ \ \theta_m\Delta^+ c_i=\theta(c_i-c_e),\ \theta_h\Delta^+\tau_i=\theta(\tau_i-\tau_e) \quad (3c)$$
$$i=N+1{:}\ \Delta^- c_i=\Delta^-\tau_i=0,\qquad (\tau_e,\theta)'=\boldsymbol{d} \quad (3d)$$
$$t=0{:}\ \ c_i(0)=c_{i0},\ \tau_i(0)=\tau_{i0},\qquad 1\le m\le N \quad (3e)$$

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 *N-stage model* is written as follows

$$\dot{\boldsymbol{x}}=\boldsymbol{f}(\boldsymbol{x},\boldsymbol{d},u),\ \boldsymbol{x}(0)=\boldsymbol{x}_0,\qquad y=\boldsymbol{c}_y\boldsymbol{x},\qquad z=\boldsymbol{c}_z\boldsymbol{x} \quad (4)$$
$$\boldsymbol{c}_y\boldsymbol{x}=\tau_m,\ \ \boldsymbol{c}_z\boldsymbol{x}=c_N,\ \ \dim\boldsymbol{x}=n=2N$$

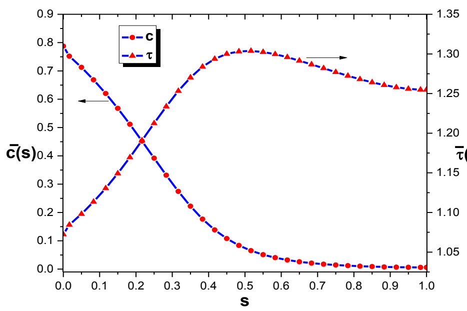

Fig. 3. Discrete approximations of the nominal open-loop unstable SS concentration and temperature profiles with $N=30$ stages (●, ▲), —: interpolation

In Fig. 3 are shown the approximations of the nominal SS profile $[\bar{c}(s),\bar{\tau}(s)]_4$ (# 4 in Fig. 2) with $N=30$ and 180 stages, showing that: (i) $N=30$ and 80 stages yield similar (root mean squared) error with respect to the "almost" distributed approximation (with $N=180$), and (ii) $N=30$

yields an adequate description of the distributed system in the light of typical kinetics-transport parameter errors.

3.2 Primary concentration FF controller

The aim is to keep the unmeasured effluent concentration z at its prescribed value $\bar{z}$ by adjusting the coolant temperature u according to the measured load disturbances $\boldsymbol{d}$, this is,

$$z(t) = c_N(t) = \bar{z} \tag{5}$$

The 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 $z(t) = \bar{z}$. In control theory, the FF control is the dynamical inverse (Hirschorn, 1979) with respect to the input-output pair (u^*, z), and its dynamic component is called the zero-dynamics (ZD) (Isidori, 1989). In industry it is known that the feedforward-feedback (FF-FB) combination is the most effective way to control a difficult process (Shinskey, 1977): the FF executes most of the disturbance rejection task, and the FB achieves stable output regulation by compensating the FF model error.

Let us rewrite the staged model (4) in the partitioned form:

$$\dot{\boldsymbol{x}}_\zeta = \boldsymbol{f}_\zeta(\boldsymbol{x}_\zeta, x_z, \boldsymbol{d}, u),\ \ \boldsymbol{x}_\zeta(0) = \boldsymbol{x}_{\zeta o},\quad y = \boldsymbol{c}_\zeta \boldsymbol{x}_\zeta = \tau_m \tag{6a}$$

$$\dot{x}_z = f_z(\boldsymbol{x}_\zeta, x_z, \boldsymbol{d}, u),\ \ x_z(0) = x_{zo},\quad z = x_z \tag{6b}$$

$$dim\,\boldsymbol{x}_\zeta = n-2,\ \ dim\,x_z = 2 = rd\,(u,z),\ \ \boldsymbol{I}_\zeta(\boldsymbol{x}_\zeta', x_z)' = \boldsymbol{x}$$

and $rd\,(u,z)$ denotes the relative degree of the input-output pair (u,z) (Isidori, 1980). The pair (u,z) has $rd = 2$ because the N-stage concentration dynamics ($\dot{c}_N$) do not depend on the coolant temperature u, and a the second time derivative ($\ddot{c}_N$) of z is needed to obtain an algebraic equation with u.

The enforcement of the regulation condition (5) followed by the solution for u of (6b) and its substitution in (6a) yields the *FF composition controller*

$$\dot{\boldsymbol{x}}_\zeta^* = \boldsymbol{f}_\zeta^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}),\ \ \boldsymbol{x}_\zeta^*(0) = \boldsymbol{x}_{\zeta_0}^*;\quad u^* = \mu^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}) \tag{7a,b}$$

$$\boldsymbol{f}_\zeta^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}) = \boldsymbol{f}_\zeta[\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}, \mu^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z})] \tag{7c}$$

with *z-minimumphase* solvability condition

$$rd(u,z) = 2 \leftrightarrow f_z\!: u\text{-invertible};\qquad \text{stable } ZD \text{ (7a)} \tag{8a,b}$$

Eq. (8a) says that the staged model (4) has $rd = 2$ for (u,z), and eq. (8b) says that the associated ZD must be stable.

3.3 Secondary FF-SF temperature tracking controller

Here the task is manipulate the coolant temperature u to track time varying setpoint y^* associated with the state $\boldsymbol{x}_\zeta^*$ of the FF controller (7a) with the prescribed linear dynamics:

$$\dot{e}_y = -ke_y,\ \ e_y = y - y^*(t),\quad y^* = \boldsymbol{c}_\zeta \boldsymbol{x}_\zeta^* \tag{9a-c}$$

where k is an adjustable gain. The enforcement of eq. (9a) on the staged model (4) followed by solution for u yields the *SF temperature tracking controller*

$$u = \mu_y(\boldsymbol{x}, \boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}) \tag{10}$$

where μ_y denotes the unique solution for u of the algebraic equation

$$f_m^\tau(\boldsymbol{x}, \boldsymbol{d}, u) = f_m^{\tau*}(\boldsymbol{x}_\zeta, \boldsymbol{d}, \bar{z}) - k_y(\boldsymbol{c}_y \boldsymbol{x} - \boldsymbol{c}_\zeta \boldsymbol{x}_\zeta^*) \tag{11}$$

$$f_m^\tau(\boldsymbol{x}, \boldsymbol{d}, u) = f_m^{\tau*}(\boldsymbol{x}_\zeta, \boldsymbol{d}, \bar{z}) = \dot{\tau}_m$$

The related *y-passivity* solvability condition is

$$rd(u,y) = 1 \leftrightarrow \boldsymbol{f}_\zeta\!: u\text{-invertible};\ SZD\ \text{(7a)} \tag{12a,b}$$

Eq. (12a) says that the staged reactor (4) has $rd = 1$ with respect to (u,y), and eq. (12b) states that the associated ZD (12b) (the ones (7a) of the primary controller (7)) must be stable. The property $rd = 1$ of (u,y) means that the temperature dynamics ($\dot{\tau}_m$) at the m-th stage depend on u.

3.4 Cascade FF-SF dynamic nonlinear controller

The combination of the primary composition (7) and secondary temperature (9) controllers yields the *composition cascade controller*

$$\dot{\boldsymbol{x}}_\zeta^* = \boldsymbol{f}_\zeta^*(\boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}),\ \ \boldsymbol{x}_\zeta^*(0) = \boldsymbol{x}_{\zeta_0}^*;\ \ u = \mu_y(\boldsymbol{x}, \boldsymbol{x}_\zeta^*, \boldsymbol{d}, \bar{z}) \tag{13a,b}$$

with z-minimum phase (8), and y-passivity (12) solvability conditions

$$rd(u,z) = 2,\quad rd(u,y) = 1,\quad \text{stable } ZD\ \text{(7a)} \tag{14a-c}$$

The negative solvability assessment of this controller and its redesign are the subjects of the next section.

4. CASCADE CONTROL REDESIGN

Here, the solvability of the FF-FB cascade controller (13) is assessed, finding that the primary control is not stable. Then the control scheme is redesigned accordingly.

4.1 Solvability of the cascade controller (13)

Introduce the eigenvalues λ_i and eigenvectors $\boldsymbol{v}_i$ of staged model (4) linearization about the nominal SS ($|\lambda_i| < |\lambda_{i+1}|$):

$$\boldsymbol{A}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i,\ i = 1, \ldots, n,\ \boldsymbol{A} = (\partial_x \boldsymbol{f})(\bar{\boldsymbol{x}}, \bar{u}, \bar{\boldsymbol{d}}) \tag{15a}$$

and denote by $\lambda_s = \lambda_1$ (or $\lambda_u < 0$) be the slowest (or unstable) eigenvalue of $\boldsymbol{A}$ and by and $\boldsymbol{v}_s$ (or $\boldsymbol{v}_u$) the corresponding eigenvector. Following studies for linear distributed systems (Ichikawa et al., 1979), the domain sensor y must be located as follows. If there is an unstable eigenvalue $\lambda_u < 0$, to ensure closed-loop stability the location m must be the node m^- (15b) where the $N+m$-th entry of $\boldsymbol{v}_u$ reaches its maximum absolute value. To attain the maximum closed-loop response, the measurement must be placed at the node m^+ (15c) where the $N+m$-th entry of $\boldsymbol{v}_1$ reaches its maximum value. This is,

$$m^- = \max_{1\le i\le N}|v_j^{u\tau}|,\qquad m^+ = \max_{1\le i\le N}|v_j^{s\tau}| \tag{15c,d}$$

where $(\sigma = s, u)$

$$(v_1^{\sigma c}, \ldots, v_N^{\sigma c})' = \boldsymbol{v}_\sigma^c,\ (v_1^{\sigma\tau}, \ldots, v_N^{\sigma\tau})' = \boldsymbol{v}_\sigma^\tau,\ (\boldsymbol{v}_\sigma^{c\prime}, \boldsymbol{v}_\sigma^{\tau\prime})' = \boldsymbol{v}_\sigma$$

The solvability conditions (14) of the cascade control (13) become

$$rd(u,z) = 2 \leftrightarrow \delta c_N \partial_\tau \alpha(\tau_N) \neq 0,\ \text{stable } ZD\ \text{(7a)} \tag{16a-b}$$

$$rd(u,y) = 1 \leftrightarrow\quad \delta \neq 0,\qquad m \in [m^-, m^+] := M \tag{16c,d}$$

While eq. (16c) (secondary control) is robustly met with sufficient heat exchange capability ($\delta > 0$), eq. (16a-b) (primary and secondary control) is not met because: (i) the nominal exit concentration $\bar{c}_N = \bar{z} \approx 0.006$ is very small

($\delta c_N \partial_\tau \alpha(\tau_N) \approx 0$), and (ii) the dynamics of the staged model with fixed $c_N = \bar{z}$ is unstable [the ZD (7a) are unstable]. Observe that the sensor location condition (16d) requires the fulfilment of the ZD stability condition (16b).

Thus, as it stands, the cascade control (13) problem: is not solvable due to the instability of its primary component (13a).

4.2 Cascade control redesign

Recall the primary controller (7) and rewrite it as

$$\dot{\boldsymbol{x}}_\zeta^* = \boldsymbol{f}_\zeta(\bar{z}, \boldsymbol{x}_\zeta^*, \boldsymbol{d}, u^*), \boldsymbol{x}_\zeta^*(0) = \boldsymbol{x}_{\zeta_0}^*; f_z(\bar{z}, \boldsymbol{x}_\zeta^*, \boldsymbol{d}, u^*) = 0$$

neglect the state accumulation ($\dot{\boldsymbol{x}}_\zeta^* = 0$), incorporate the temperature setpoint map (9c), replace $(\boldsymbol{x}_\zeta^*, u^*)$ by $(\boldsymbol{x}_\zeta^s, u_s)$,

$$\boldsymbol{f}_\zeta(\bar{z}, \boldsymbol{x}_\zeta^*, \boldsymbol{d}, u^*) = 0,\ f_z(\bar{z}, \boldsymbol{x}_\zeta^*, \boldsymbol{d}, u^*) = 0,\ y^* = \boldsymbol{c}_\zeta \boldsymbol{x}_\zeta^* \quad \text{(17a-c)}$$

and rewrite (17) as follows

$$(\boldsymbol{x}_\zeta^{s\prime}, u_s)' = \boldsymbol{\sigma}(\boldsymbol{d}, \bar{z}), \qquad y_s = \boldsymbol{c}_\zeta \boldsymbol{x}_\zeta^s = \boldsymbol{c}_\zeta \sigma_{x_\zeta}(\boldsymbol{d}, \bar{z}) \coloneqq \phi(\boldsymbol{d}, \bar{z})$$

where $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_{x_\zeta}', \sigma_u)'$ denotes the unique solution for $(\boldsymbol{x}_\zeta^s, u_s)$ of (7a-b). Pick the last component and add a first order lag (18b) to compensate the effect of the no-accumulation assumption ($\dot{\boldsymbol{x}}_\zeta^* = 0$), and obtain the *setpoint compensator*

$$y_s = \phi(\boldsymbol{d}, \bar{z});\ \dot{y}^* = -k_*(y^* - y_s),\ y^*(0) = y_0^*,\ k_* \approx \lambda_y \quad \text{(18a,b)}$$

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

$$\det J(\boldsymbol{x}_\zeta^s, \boldsymbol{d}, u_s) \neq 0 \quad (19)$$

is the z-passivity, with $rd = 0$ (Khalil, 2002) for $(\bar{z}, y_s)$, of the static component (18a). Since the dynamic component (18b) is passive, with $rd = 1$ for (y_s, y^*), the setpoint compensator (18) is passive with respect to $(\bar{z}, y^*)$.

The combination of the primary (18) and secondary (10) controllers yields the *redesigned stable dynamic cascade controller*

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

$$u = \mu(\boldsymbol{x}, \boldsymbol{d}, u, y^*, y_s) \quad \text{(20c)}$$

where μ denotes the unique solution for u of the equation

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

The corresponding solvability conditions are:

$$det\, J(\boldsymbol{x}_\zeta^s, \boldsymbol{d}, u_s) \neq 0, \quad \delta \neq 0,\ \ m \in M \quad \text{(21a-c)}$$

5. FF-OF CONTROLLER

The combination of the passivated cascade controller (18) with a geometric observer, with second-order detectability innovation structure (Fernandez et al., 2012) because $\beta\alpha(\tau) \neq 0$, yields the *robust FF-OF controller*

$$\dot{y}^* = -k_*(y^* - y_s), y^*(0) = y_0^*; y_s = \phi(\boldsymbol{d}, \bar{z}) \quad \text{(22a,b)}$$

$$\dot{\hat{\boldsymbol{x}}} = \boldsymbol{f}(\hat{\boldsymbol{x}}, \boldsymbol{d}, u) + \boldsymbol{g}_y(\hat{\boldsymbol{x}}, u)(y - \boldsymbol{c}_y \hat{\boldsymbol{x}}) + \boldsymbol{g}_\iota(\hat{\boldsymbol{x}}, u)\hat{\iota} \quad \text{(22c)}$$

$$\dot{\hat{\iota}} = \omega_y^3(y - \boldsymbol{c}_y \hat{\boldsymbol{x}}),\ \hat{\iota}(0) = \hat{\iota}_o, \qquad \hat{\boldsymbol{x}}(0) = \hat{\boldsymbol{x}}_o \quad \text{(22d)}$$

$$u = \mu(\hat{\boldsymbol{x}}, \boldsymbol{d}, u, y^*, y_s), \qquad \zeta_y[1,3],\ \omega_y \in [5,10]\lambda_y \quad \text{(22e)}$$

where $dim(y^*, \hat{\boldsymbol{x}}', \hat{\iota})' = n + 3 = 63, \quad n = 2N = 60$

$$\boldsymbol{g}_i(\boldsymbol{x}, \boldsymbol{d}, u) = [\boldsymbol{0}', \boldsymbol{O}^{-1\prime}(\boldsymbol{x}, \boldsymbol{d}, u)\boldsymbol{k}_i, \boldsymbol{0}']', \quad i = y, \iota$$

$$\boldsymbol{O}(\boldsymbol{x}, \boldsymbol{d}, u) = \partial_{x_\iota}\boldsymbol{\varphi}(\boldsymbol{x}, \boldsymbol{d}, u),\ \ \boldsymbol{\varphi}(\boldsymbol{x}, \boldsymbol{d}, u) = [\tau_m, f_m^\tau(\boldsymbol{x}, \boldsymbol{d}, u)]'$$

$$\boldsymbol{k}_y = (2\zeta_y + 1)(\omega_y, \omega_y^2)',\ \boldsymbol{k}_\iota = (0,1)'$$

$\boldsymbol{g}_y$ (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 solvability conditions are:

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

The sensor location criteria (21c) for the secondary control (22e) coincides with the one for state estimation (22c-d) (Fernandez et al., 2012). As we shall see in Section 7, this in agreement criteria of previous control studies and industrial practice (Harris et al., 1980).

However, with respect to our application-oriented design specification, the dynamic controller FF-OF controller (22) for the distributed tubular reactor (1) is too complex: highly nonlinear, interactive and made of $2N + 2$ ODEs (62 for the case example). The tackling of this complexity obstacle is the subject of the next section.

6. PI TEMPERATURE CONTROLLER WITH DYNAMIC FF SETPOINT COMPENSATION

Here, the behavior of the staged model-based robust FF-OF controller (22) is recovered with a simplified controller built according to passivity and observability properties: a PI controller with antiwindup protection and FF dynamic setpoint compensation.

6.1 Secondary controller redesign

Let us recall the N-stage model (4) and express its y-output dynamics in the form (Gonzalez and Alvarez, 2005)

$$\dot{y} = -au + \iota; \qquad \iota = f_m^\tau(\boldsymbol{x}, \boldsymbol{d}, u) + au, \qquad a \approx \bar{a} \quad \text{(24a,b)}$$

$$rd(u, y) = rd(\iota, y) = 1, \quad \bar{a} = (\partial_u f_m^\tau)(\bar{\boldsymbol{x}}, \bar{\boldsymbol{d}}, \bar{u}) > 0$$

f_m^τ is defined after (11), ι is an observable input, and (u, ι) satisfies the matching condition (meaning robustness for control design) (Sepulchre, 2011). The elimination of the static nonlinear component (24b) in eq. (24) yields the *simplified model*

$$\dot{y} = -au + \iota, \qquad rd(u, y) = rd(\iota, y) = 1 \quad \text{(25a,b)}$$

for temperature control design, with unmeasured-observable input ι. The enforcement of the tracking condition (9) upon this model yields the secondary controller (10) in the ι-dependent form (26a), and a convergent estimate $\hat{\iota}$ of input ι of model (25) is given by the reduced-order observer (26b) with adjustable (up to measurement noise) exponential convergence rate ω (Gonzalez and Alvarez, 2005):

$$u = [k_*(y^* - y_s) + k(y - y^*) + \iota]/a \quad \text{(26a)}$$

$$\dot{\chi} = -\omega\chi - \omega(\omega y - au),\ \chi(0) = 0,\ \hat{\iota} = \chi + \omega y \quad \text{(26b)}$$

The combination of control (26a) (with $\iota = \hat{\iota}$) with observer (26b) yields the dynamic *temperature tracking controller*

$$\dot{\chi} = -\omega\chi - \omega(\omega y - au), \qquad \chi(0) = 0 \quad \text{(27a)}$$

$$u = [k_*(y^* - y_s) + \omega y^* + (k + \omega)(y - y^*) + \chi]/a \quad \text{(27b)}$$

with one linear ODE, and similar behavior than the one (22c,e) of its detailed model-based counterpart (22) with $2N+2$ ODEs.

6.2 PI temperature controller with FF setpoint compensation

The combination of the primary (22a-b) and redesigned secondary (27) control yields the *simplified FF-OF control*:

$$\dot{y}^* = -k_*(y^* - y_s),\ y_s = \phi(\boldsymbol{d}, \bar{z})\ (\boldsymbol{d}\text{ -feedforward}) \quad (28a,b)$$
$$\dot{\chi} = -\omega\chi - \omega(\omega y - au),\quad \chi(0) = 0\ (y\text{-feedback}) \quad (28c)$$
$$u = [k_*(y^* - y_s) + \omega y^* + (k+\omega)(y - y^*) + \chi]/a \quad (28d)$$

with: (i) two linear ODEs, and (ii) and similar behavior than the one (22c,e) of its detailed model-based counterpart (22) with $2N+3$ ODEs (63 for case example). This control has antiwindup protection because the χ-dynamics (28c) runs regardless of control saturation.

For applicability and comparison purposes, assume there is no saturation and express controller (28) in PI form

$$\dot{y}^* = -k_*(y^* - y_s),\qquad y_s = \phi(\boldsymbol{d}, \bar{z}) \quad (29a)$$
$$u_f = \bar{u} + k_*(y^* - y_s),\qquad u = u_f + \pi(y - y^*) \quad (29b)$$

where

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

and κ (or τ) is the proportional gain (or reset time). This signifies that the proposed controller (28) is an upgraded version the conventional PI:

$$u = \bar{u} + \pi(y - y^*) \quad (30)$$

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 FUCNTIONING

The FF-OF controller (28) is tested compared with the PI (30) with fixed set-point, for the case example (2) with $N = 30$-stage model (4). The objective is to regulate with robust closed-loop stability the exit concentration $z \approx \bar{z} = 0.006$ of the open-loop unstable SS $[\bar{c}(s), \bar{\tau}(s)]_4$ (Fig. 2).

7.1 Sensor location

The slowest and unstable eigenvalues coincide $\lambda_u = \lambda_s$, implying that $m = m^- = m^+$). In Fig. 4 are plotted the entries of the temperature vector $\boldsymbol{v}_s^\tau$ associated to the eigenvector $\boldsymbol{v}_s$, showing that: the measurement must be located at stage $m = 8$ of the $N = 30$-stage model (4), or equivalently at length $s_m \sim 0.25$ of the distributed reactor (1). In Fig. 4 are also plotted the temperature concavity $\partial_{ss}\tau$ of the distributed system (1), and the gradient $\Delta^+\tau_i$ of the staged one (4), showing that: the measurement must be located at: (i) the maximum m of $v_i^{s\tau}$ of the staged system (1), (ii) the maximum of the temperature gradient ($\partial_s\tau = 0$) of the distributed model (1) before the hot spot [in agreement with previous studies and control practice (Bashir et al. 1992), and (iii) at the stage of maximum temperature gradient ($\Delta^2\tau_i \approx 0$) before the hot spot of the staged system (in agreement with sensor location criteria for multicomponent distillation columns (Porru et al., 2014).

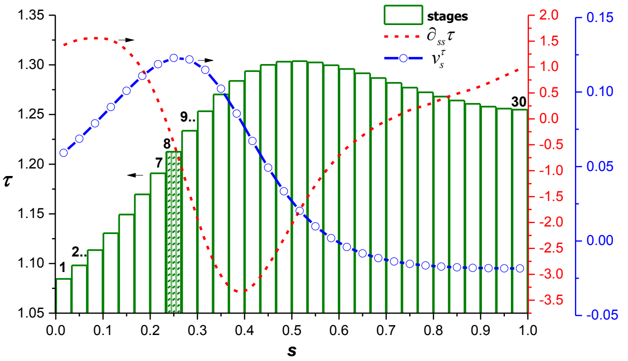

Fig 4. Temperature eigenvector $v_i^{s\tau}$ (○), gradient $\Delta^+\tau_i$ (□) sequences of the staged model (4) with $N = 30$, concavity $\partial_{ss}\tau$ (- -) of the distributed model (1), and sensor location: $m = \max_{1\le i\le N}(v_i^{s\tau}) = 8$ in (4) $\cong s_m \sim 0.25$ in (1).

Thus, the proposed eigenvector-based sensor location criterion: (i) constitute an advanced control version of the previous insight and testing-based ones employed in previous reactor studies, and (ii) interestingly, coincide with the ones employed in distillation column control.

7.2 FF static component

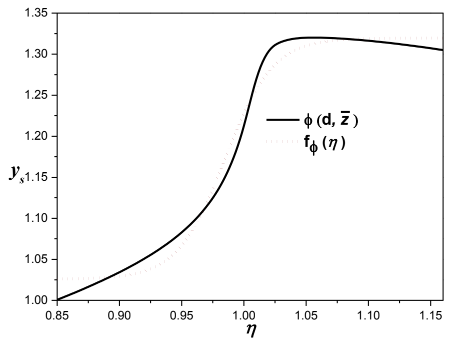

Fig.5. Static component $y_s = \phi(\boldsymbol{d}, \bar{z})$ of the setpoint compensator: computed (—) with $N = 30$ stages and fitted (••••) with eq. (31d).

$$y_s = \phi(\boldsymbol{d}, \bar{z}) \approx \hat{\phi}(\boldsymbol{d});\ \hat{\phi}(\boldsymbol{d}) = f_\phi(\eta);\ \eta = \theta\tau_e \quad (31a\text{-}c)$$
$$f_\phi(\eta) = a_2 + (a_1 - a_2)/[1 + \exp[(\eta - a_3)/a_4] \quad (31d)$$

where: $(a_1, a_2, a_3, a_4) = (1.026, 1.32, 0.985, 0.019)$

The asymmetry of ϕ reflects the strong parametric sensitivity of the nominal steady-state: a $+5°$ feed temperature increase yields a $\approx +30°$ temperature setpoint increase.

7.3 Control functioning

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) ($\lambda_y \approx q \approx 1$: open-loop characteristic time)

$$k_* = \lambda_y,\quad k = n_y\lambda_y,\quad \omega = n_\omega k,\quad n_y = 3,\quad n_\omega = 5$$

In Fig. 6 are presented the behaviors of the standard (with fixed setpoint) (29b) and proposed (with setpoint compensation) (28) controllers when the reactor is subjected to a sequence of step changes, showing that the proposed controller (28): (i) robustly stabilizes the reactor, and (ii) in comparison to its standard PI counterpart (29b), reduces by ≈ 70% the upper variability bound of the exit concentration.

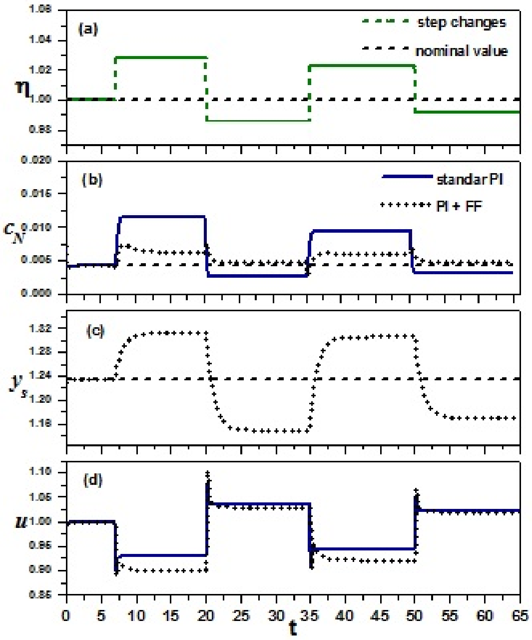

Fig.6 Closed-loop behavior with PI temperature control and feed temperature step disturbances (a), with (••••) and without (—) setpoint compensation.

8. CONCLUSIONS

The problem of regulating with robust closed-loop stability the effluent concentration of an open-loop unstable tubular reactor has been addressed. Advanced control theory was applied: (i) to develop an N-stage model-based FF-OF robust stabilizing controller with a large number $(2N+3)$ 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 of the standard PI temperature controller employed in industrial practice, with the upgrade consisting in: (i) efficient tuning/retuning with antiwindup protection, and (ii) dynamic setpoint compensation driven in FF manner by the measured load disturbances. The FF compensator had a precomputed N-stage model-based nonlinear static component with an on-line linear first-order lag. It was demonstrated that the staged model approach offers a tractable means to address control and estimation problems in highly nonlinear tubular reactors.

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