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# Control of an exothermic packed-bed tubular reactor

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Abstract: The problem of robustly controlling a highly exothermic gas-phase packed-bed tubular reactor on the basis of feed and reactor temperature measurements is addressed. First, advanced nonlinear control yields a detailed model-based output feedback (OF) control design with passivity and observability solvability conditions, sensor location criterion, and simple tuning. Then, the behavior of the advanced controller is recovered with a simplified model-based realization that amounts to an industrial temperature tracking controller with feedforward (FF) dynamic setpoint compensation. The advanced and industrial controllers are formally connected. The approach is illustrated and tested with a representative case example through numerical simulations.



*Keywords:* packed bed tubular reactor, staged model, feedforward control, output-feedback control, setpoint compensation, passive control, PI control.

## 1. INTRODUCTION

An important class of industrial processes (like oxidation of ethylene, naphthalene, vinyl acetate synthesis and hydrogenation) take place in highly exothermic gas-phase catalytic fixed packed bed (FPB) tubular reactors. These reactors: (i) consist of a compact, immobile stack of randomly arranged catalyst pellets that are bathed by the (gas) reactant fluid, which reacts over the (interior or exterior) catalyst surface (Rase, 1990; Jakobsen, 2008), (ii) are relatively easy to maintain, and produce high per-volume conversion, but (iii) rises a difficult control problem due to complex nonlinear dynamics (spatially distributed, multiplicity, parametric sensitivity, nonminimum phase characteristics, limit cycling, and structural instability) (Jensen et al., 1982; Jorgensen, 1986).

Basically, FPB reactors are controlled by adjusting the heat extraction rate according to a temperature PI controller driven by a sensor at the most sensitive axial location (Bashir et al., 1992; Jaisathaporn et al., 2004; Del Vecchio et al., 2005). The effect of measured disturbances are compensated by adjusting the temperature setpoint with a diversity of procedures that range from manual to model-based (Brosilow & Joseph, 2002).

The PI controllers are robust and cheap, but their design and supervision rely heavily on per-reactor characteristics and experience. The related setpoint compensation is done with heuristic procedures (Aguilar-López, 2007; Akamatsu et al., 2000). This motivates the development of systematic ways to design robustly stabilizing temperature controllers with feedforward-based disturbance rejection capability.

In this study, the problem of robustly controlling an exothermic FPB tubular reactor is addressed by combining advanced and industrial control ideas. Advanced control is applied to assess solvability and draw a detailed model-based nonlinear geometric OF control solution. On the basis of passivity and observability properties in the light of industrial control requirements, the behavior of the advanced nonlinear OF controller is recovered with a linear PI temperature controller equipped with model-based (preprogrammed) setpoint compensation. The methodology is illustrated and tested with a case example through numerical simulations.

## 2. CONTROL PROBLEM

Let us consider the jacketed FPB tubular reactor, depicted in Fig. 1, where a gas stream is fed (with molar flow $W_e$, temperature $T_e$, and molar composition $\chi_e$) and converted into product (at reactant composition $\chi$ and temperature $T$) by means of a reaction rate ($R$).

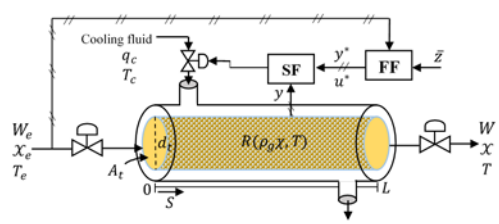


Fig. 1. FPB tubular reactor and its control scheme

Under standard assumptions (ideal gas, only axial spatial distribution, quasi-static gas phase concentration, low pressure drop, negligible mass axial dispersion and heat radiation, as well as negligible intra-solid and gas-solid transport resistance) (Hlavacek, 1970; Rase, 1990), the reactor dynamics are given by the spatially distributed dynamic mass and heat balances

$$0 = -w\partial_s c - r(c,\tau),\ 0 < s \leq 1;\ z = c(1,t) \qquad \text{(1a-b)}$$

$$\partial_t \tau = \delta\partial_{ss}\tau - w\partial_s\tau + r(c,\tau) - \upsilon(\tau - u) \qquad \text{(1c-d)}$$

$$0 < s < 1;\quad y = \tau(s_m, t),\quad s_m \in M$$

with boundary and initial conditions


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$$s = 0: \quad c(0,t) = c_e, \quad \delta\partial_s\tau = w(\tau - \tau_e) \qquad \text{(1e-f)}$$
$$s = 1: \quad \partial_s\tau = 0; \qquad t = 0: \quad \tau(s,0) = \tau_0(s) \qquad \text{(1g-h)}$$

where

$$u = \tau_c, \qquad w = q_e/\tau_e, \qquad d = \tau_e$$
$$c = \chi/\chi_r, \; c_e = \chi_e/\chi_r, \; \tau = T/T_r, \; \tau_e = T_e/T_r, \; \tau_c = T_c/T_r$$
$$q_e = Q_e/Q_r, \; t = t_a/t_r, \quad t_r = C_s/(\theta_r\rho_{gr}Cp_g)$$
$$T_r = (-\Delta H)\chi_r/Cp_g, \quad \theta_r = q_r/V, \quad \upsilon = UAt_r/(VC_s)$$
$$r(c,\tau) = R(\rho_{gr}\chi_r c, T_r\tau)/R_r, \qquad R_r = R(\rho_{gr}\chi_r, T_r)$$
$$Da = (1-\epsilon)R_r/(\rho_{gr}\chi_r\theta_r), \qquad \delta = D_h/(L^2\theta_r)$$

$c(s,t)$ [or $\tau(s,t)$] is the composition (or temperature) time-varying spatial profile, $t$ is the time, $s$ is the axial length, $c_e$ is the (nearly constant) feed composition, $\delta$ is the (Peclet inverse) heat dispersion number, $\upsilon$ is the heat transfer parameter, $w$ is the molar feed rate, $r(c,\tau)$ is the reaction rate, and $Da$ is the Damköhler number. The exit gas composition ($z$) is the *regulated output*, the cooling jacket temperature ($u$) is the *manipulated input*, the measured output is the temperature ($y$) at axial location $s_m$ to be determined, and the feed temperature $\tau_e$ is the *measured disturbance* ($d$).

As *case study*, let us consider reactor (1) with an irreversible first-order exothermic reaction $r(c,\tau)$ with Arrhenius temperature dependency (2a), the parameters (2b) and nominal inputs (2c):

$$r(c,\tau) = c\alpha(\tau), \quad \alpha(\tau) = (1/\tau)\exp(a - \gamma/\tau) \qquad \text{(2a)}$$
$$a = \ln(Da) = 25, \quad \gamma = 50, \quad \delta = 0.4, \quad \upsilon = 3 \qquad \text{(2b)}$$
$$\bar{c}_e = \bar{q}_e = 1, \quad \bar{w} = 0.57, \quad \bar{\tau}_e = 1.75, \quad \bar{\tau}_c = 2 \qquad \text{(2c)}$$

This corresponding reactor (1): (i) has the single stable steady-state profile pair $[\bar{c}(s), \bar{\tau}(s)]$ shown in Fig. 2 (drawn with a 200-staged model plus interpolation), and (ii) exhibits strong parametric sensitivity with temperature hotspot at length $\approx 0.15$ .

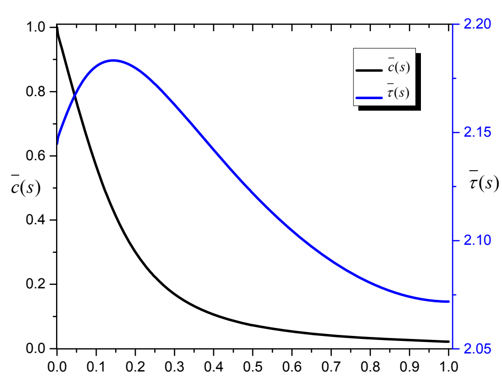


Fig. 2. Steady-state composition-temperature profile pair.

The *problem* consists in designing an feedforward-output feedback (FF-OF) robust controller for reactor (1) that manipulates the coolant temperature $u$ on the basis of the feed input disturbance ($d$) and output temperature ($y$) measurements, so that the exit gas composition $z$ is indirectly regulated about its prescribed value $\bar{z}$, and the temperature profile is regulated about a compensated setpoint ($y^*$).

## 3. FF-SF CONTROL

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

### 3.1 Staged model

Following studies that use staged models to describe tubular reactors (Deckwer, 1974; Badillo-Hernandez et al., 2013; Nájera et al. 2015), the application of spatial finite differences (with $N$ domain nodes and two boundary ones) to the distributed reactor (1) yields the pair of static-dynamic spatial difference equations

$$0 = -\theta_m\Delta^-c_i - r(c_i,\tau_i), \qquad 1 \le i \le N; \qquad z = c_N \qquad \text{(3a-b)}$$
$$\dot{\tau}_i = \theta_h\Delta^2\tau_i - \theta_m\Delta^-\tau_i + r(c_i,\tau_i) - \upsilon(\tau_i - u); \; y = \tau_m \qquad \text{(3c-d)}$$
$$i = 0: \quad c_i = c_e; \qquad \theta_h\Delta^+\tau_i = \theta_m(\tau_i - \tau_e) \qquad \text{(3e-f)}$$
$$i = N+1: \qquad \Delta^-\tau_i = 0; \quad d = \tau_e \qquad \text{(3g-h)}$$
$$t = 0: \quad \tau_i(0) = \tau_{io}; \qquad m \in M = \{1,\dots,N\} \qquad \text{(3i-j)}$$

where

$$\theta_h = N^2\delta, \quad \theta_m = Nw$$
$$\Delta^-(\cdot)_i = (\cdot)_i - (\cdot)_{i-1}, \qquad \Delta^+(\cdot)_i = (\cdot)_{i+1} - (\cdot)_i$$
$$\Delta^2(\cdot)_i = (\cdot)_{i+1} - 2(\cdot)_i + (\cdot)_{i-1}$$

In compact notation, eq. (3) is written as

$$0 = \boldsymbol{\varphi}_c(\boldsymbol{c},\boldsymbol{x}); \qquad z = \boldsymbol{c}_z\boldsymbol{c} \qquad \text{(4a-b)}$$
$$\dot{\boldsymbol{x}} = \boldsymbol{\varphi}_\tau(\boldsymbol{c},\boldsymbol{x},u,d), \quad \boldsymbol{x}(0) = \boldsymbol{x}_o; \quad y = \boldsymbol{c}_y\boldsymbol{x} \qquad \text{(4c-d)}$$
$$\boldsymbol{c}_y\boldsymbol{x} = \tau_m, \quad \boldsymbol{c}_z\boldsymbol{c} = c_N, \quad \dim\boldsymbol{\kappa} = \dim\boldsymbol{x} = N \qquad \text{(4e-g)}$$

where

$$\boldsymbol{x} = (\tau_1,\dots,\tau_N)^T, \; \boldsymbol{c} = (c_1,\dots,c_N)^T$$

The unique solution [$\boldsymbol{c} = \boldsymbol{h}(\boldsymbol{x})$] for the composition vector $\boldsymbol{c}$ of eq. (4a) followed by substitution in the heat balance (4c) yields the *N-dimensional staged model*

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x},u,d), \qquad \boldsymbol{x}(0) = \boldsymbol{x}_o, \quad \dim\boldsymbol{x} = \boldsymbol{c} = N \qquad \text{(5a-b)}$$
$$\boldsymbol{c} = \boldsymbol{h}(\boldsymbol{x}); \qquad z = \boldsymbol{c}_z\boldsymbol{c}; \qquad y = \boldsymbol{c}_y\boldsymbol{x} \qquad \text{(5c-e)}$$

with dynamic (or quasi-static) temperature $\boldsymbol{x}$ (or composition $\boldsymbol{c}$) sequence, where

$$\boldsymbol{f}(\boldsymbol{x},u,d) = \boldsymbol{\varphi}_\tau[\boldsymbol{h}(\boldsymbol{x}),\boldsymbol{x},u,d]$$

In Fig. 3 the van Heerden (van Heerden, 1958) diagram (heat generated $Q_g$ and removed $Q_r$ versus 1st stage temperature $\tau_1$) for Example (2) is presented for $N = 10$ and $200$ stages, showing that: (i) in both cases the staged model has one stable steady-state (SS) ($\bar{\boldsymbol{x}}$), and (ii) the SS with $N = 10$ approximates well (up to admissible deviation) the one with $N = 200$.

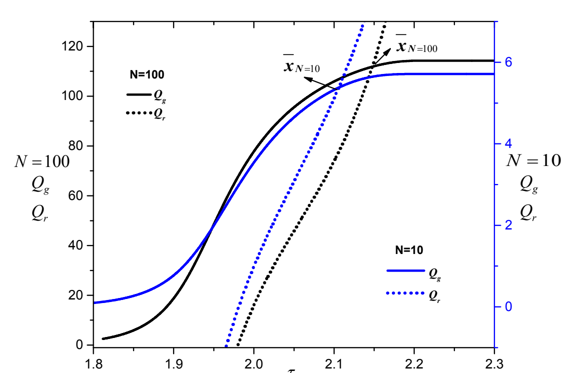


Fig. 3. Reactor SS uniqueness according to van Herden diagram, on the basis of the $N$ (— 100 and — 10)-staged model (5).