

CASCADE CONTROL OF A TUBULAR CHEMICAL REACTOR USING NONLINEAR PART OF PRIMARY CONTROLLER

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KEYWORDS

Cascade control, tubular chemical reactor, external linear control, pole assignment.

ABSTRACT

The paper deals with the cascade control of a tubular chemical reactor. The control is performed in the primary and secondary control-loops. A gain of the primary discrete nonlinear P controller consists of two parts. The first nonlinear part is determined on the basis of simulated or measured steady-state characteristics of the reactor, the second part is selectable. The controller in the secondary control-loop is an adaptive controller. The proposed method is verified by control simulations on a nonlinear model of the reactor with an exothermic reaction.

INTRODUCTION

The cascade control belongs to useful control methods for many technological processes. It may be applied in such cases when at least two output variables can be measured and only one input variable is available to the control. Principles and examples of the use of cascade control can be found e.g. in (Smuts 2011; King 2010; Seborg et al. 1989).

Chemical reactors are typical processes suitable for the use of cascade control. In cases of non-isothermal reactions, concentrations of the reaction products mostly depend on a temperature of the reactant. Further, it is known that while the reactant temperature can be measured almost continuously, concentrations are usually measured in longer time intervals. Then, the application of the cascade control method can lead to good results. In this paper, the procedure for control design of a tubular chemical reactor is presented.

Tubular chemical reactors (TCRs) are units frequently used in chemical industry inclusive of manufacturing and processing of polymers and some others. From the system theory point of view, TCRs belong to the class of nonlinear distributed parameter systems. Their mathematical models are described by sets of nonlinear partial differential equations (PDEs). The methods of modelling and simulation of such processes are described e.g. in (Corriou 2004; Ingham et al. 1994). Detailed analysis of the specific TCR is carried out for example in (Dostál et al. 2008).

In this paper, the TCR control strategy is based on the fact that a concentration of the main component of the reaction taking place in the reactor depends on the output reactant temperature. Moreover, the procedure assumes that the output reactant temperature is measured continuously. Then, in the cascade control-loop, the concentration of a main product of the reaction is considered as the primary controlled variable, and, the output reactant temperature as the secondary controlled variable. The coolant flow rate represents a common control input. The primary controller determining the set point for the secondary (inner) control-loop is derived as a proportional controller with a nonlinear part obtained from the steady-state characteristics of the reactor and with a selectable part. Since the controlled process is nonlinear, a continuous-time adaptive controller is used as the secondary controller. The procedure for the adaptive control design in the inner control-loop is based on approximation of a nonlinear model of the TCR by a continuous-time external linear model (CT ELM) with recursively estimated parameters. In the process of the parameter estimation, a corresponding delta model is used, see, e.g. (Garnier and Wang 2008; Mukhopadhyay et al. 1992; Stericker and Sinha 1993; Bobál et al. 2005). The resulting CT controller is derived on the basis of the polynomial method, see, e.g. (Kučera 1993; Mikleš and Fikar 2004; Dostál et al. 2007). The control is tested by simulations on nonlinear model of the TCR with a consecutive exothermic reaction.

MODEL OF TCR

An ideal plug-flow tubular chemical reactor with a simple exothermic consecutive reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ in the liquid phase and with the countercurrent cooling is considered. Heat losses and heat conduction along the metal walls of tubes are assumed to be negligible, but dynamics of the metal walls of tubes are significant. All densities, heat capacities, and heat transfer coefficients are assumed to be constant. Under above assumptions, the reactor model is described by five PDEs in the form

$$\frac{\partial c_A}{\partial t} + v_r \frac{\partial c_A}{\partial z} = -k_1 c_A \quad (1)$$

$$\frac{\partial c_B}{\partial t} + v_r \frac{\partial c_B}{\partial z} = k_1 c_A - k_2 c_B \quad (2)$$

$$\frac{\partial T_r}{\partial t} + v_r \frac{\partial T_r}{\partial z} = \frac{Q_r}{(\rho c_p)_r} - \frac{4U_1}{d_1(\rho c_p)_r} (T_r - T_w) \quad (3)$$

$$\frac{\partial T_w}{\partial t} = \frac{4}{(d_2^2 - d_1^2)(\rho c_p)_w} [d_1 U_1 (T_r - T_w) + d_2 U_2 (T_c - T_w)] \quad (4)$$

$$\frac{\partial T_c}{\partial t} - v_c \frac{\partial T_c}{\partial z} = \frac{4n_1 d_2 U_2}{(d_3^2 - n_1 d_2^2)(\rho c_p)_c} (T_w - T_c) \quad (5)$$

with initial conditions

$$c_A(z, 0) = c_A^s(z), \quad c_B(z, 0) = c_B^s(z), \quad T_r(z, 0) = T_r^s(z),$$

$$T_w(z, 0) = T_w^s(z), \quad T_c(z, 0) = T_c^s(z)$$

and boundary conditions

$$c_A(0, t) = c_{A0}(t) \text{ (kmol/m}^3\text{)}, \quad c_B(0, t) = c_{B0}(t) \text{ (kmol/m}^3\text{)},$$

$$T_r(0, t) = T_{r0}(t) \text{ (K)}, \quad T_c(L, t) = T_{cL}(t) \text{ (K)}.$$

Here, t is the time, z is the axial space variable, c stands for concentrations, T for temperatures, v for fluid velocities, d for diameters, ρ for densities, c_p for specific heat capacities, U for heat transfer coefficients, n_1 is the number of tubes and L is the length of tubes. The subscript $(\cdot)_r$ stands for the reactant mixture, $(\cdot)_w$ for the metal walls of tubes, $(\cdot)_c$ for the coolant, and the superscript $(\cdot)^s$ for steady-state values.

The reaction rates and heat of reactions are nonlinear functions expressed as

$$k_j = k_{j0} \exp\left(\frac{-E_j}{RT_r}\right), \quad j = 1, 2 \quad (6)$$

$$Q_r = (-\Delta H_{r1}) k_1 c_A + (-\Delta H_{r2}) k_2 c_B \quad (7)$$

where k_0 are pre-exponential factors, E are activation energies, $(-\Delta H_r)$ are reaction enthalpies in the negative consideration and R is the gas constant.

The fluid velocities are calculated via the reactant and coolant flow rates as

$$v_r = \frac{4q_r}{\pi n_1 d_1^2}, \quad v_c = \frac{4q_c}{\pi (d_3^2 - n_1 d_2^2)} \quad (8)$$

The TCR parameter values with correspondent units used for simulations are given in Table 1.

From the system engineering point of view, $c_A(L, t) = c_{Aout}$, $c_B(L, t) = c_{Bout}$, $T_r(L, t) = T_{rout}$ and $T_c(0, t) = T_{cout}$ are the output variables and $q_r(t)$,

$q_c(t)$, $c_{A0}(t)$, $T_{r0}(t)$ and $T_{cL}(t)$ are the input variables. Among them, for the control purposes, mostly the coolant flow rate can be taken into account as the control variable, whereas other inputs entering into the process can be accepted as disturbances. In this paper, the output reactant temperature

$$T_{rout} = T_r(L, t) \quad (9)$$

is considered as the secondary (inner) controlled output. The concentration c_{Bout} represents the primary controlled output.

TABLE I: VARIABLES USED IN CONTROL AND APPROXIMATIONS

$L = 8 \text{ m}$	$n_1 = 1200$
$d_1 = 0.02 \text{ m}$	$d_2 = 0.024 \text{ m}$
$d_3 = 1 \text{ m}$	
$\rho_r = 985 \text{ kg/m}^3$	$c_{pr} = 4.05 \text{ kJ/kg K}$
$\rho_w = 7800 \text{ kg/m}^3$	$c_{pw} = 0.71 \text{ kJ/kg K}$
$\rho_c = 998 \text{ kg/m}^3$	$c_{pc} = 4.18 \text{ kJ/kg K}$
$U_1 = 2.8 \text{ kJ/m}^2\text{s K}$	$U_2 = 2.56 \text{ kJ/m}^2\text{s K}$
$k_{10} = 5.61 \cdot 10^{16} \text{ 1/s}$	$k_{20} = 1.128 \cdot 10^{18} \text{ 1/s}$
$E_1/R = 13477 \text{ K}$	$E_2/R = 15290 \text{ K}$
$(-\Delta H_{r1}) = 5.8 \cdot 10^4 \text{ kJ/kmol}$	$(-\Delta H_{r2}) = 1.8 \cdot 10^4 \text{ kJ/kmol}$
$c_{A0}^s = 2.85 \text{ kmol/m}^3$	$c_{B0}^s = 0 \text{ kmol/m}^3$
$T_{r0}^s = 323 \text{ K}$	$T_{cL}^s = 293 \text{ K}$
$q_r^s = 0.15 \text{ m}^3/\text{s}$	

COMPUTATION MODELS

For computation of both steady-state and dynamic characteristics, the finite differences method is employed. The procedure is based on substitution of the space interval $z \in \langle 0, L \rangle$ by a set of discrete node points $\{z_i\}$ for $i = 1, \dots, n$, and, subsequently, by approximation of derivatives with respect to the space variable in each node point by finite differences. The procedure is in detail described in (Dostál et al. 2008).

THE CONTROL OBJECTIVE AND STEADY-STATE CHARACTERISTICS

Basic scheme of the cascade control is in Fig. 1. Here, NPC stands for the nonlinear proportional controller, AC for the adaptive controller.

The control objective is to achieve a concentration of the component B as the primary controlled output near to its maximum. A dependence of the concentration of B on the output reactant temperature is in Fig. 2.

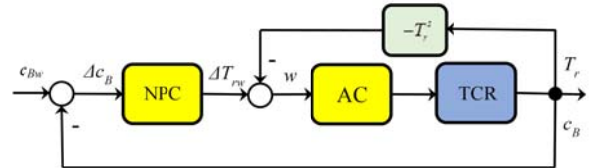


Figure 1: Cascade Control Scheme.

There, an operating interval consists of two parts. In the first subinterval, the concentration B increases with increasing reactant temperature, in the second subinterval it again decreases. The endpoints defining both intervals are

$$315.55 \leq T_{rout} \leq 328.49 \quad 1.344 \leq c_B^s \leq 2.2$$

in the first interval, and,

$$331.32 \leq T_{rout} \leq 334.63 \quad 1.356 \leq c_B^s \leq 2.2$$

in the second interval.

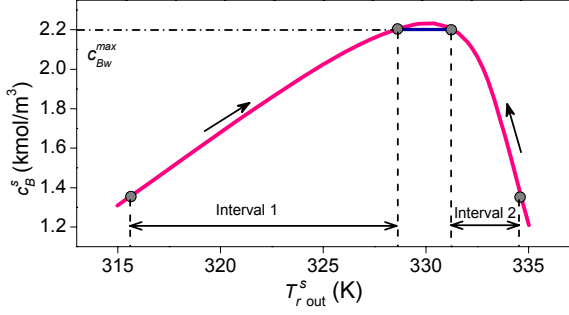


Figure 2: Steady-State Dependence of Product B Concentration on Output Reactant Temperature.

It can be seen in Fig. 2 that the maximum value of c_B can be slightly higher than 2.2 kmol/m^3 . However, the maximum desired value of c_B will be limited just by 2.2 kmol/m^3 .

For purposes of later approximations, the output temperature is transformed as

$$\xi = \frac{T_{r,out} - T_{r,out}^{\min}}{T_{r,out}^{\max} - T_{r,out}^{\min}} \quad (10)$$

where $T_{r,out}^{\min} = 315.46$ and $T_{r,out}^{\max} = 335.01$.

The dependence of c_B on ζ is shown in Fig. 3.

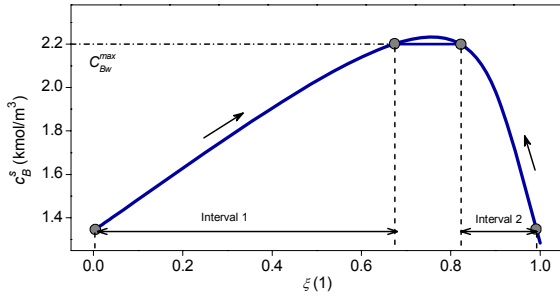


Figure 3: Steady-State Dependence of c_B on ζ .

THE NPC DESIGN

The procedure of the NPC design appears from steady-state characteristics and its subsequent polynomial approximation. Steady-state characteristics with polynomial approximations corresponding with Fig. 3 can be seen in Figs. 4 and 5.

The polynomials for both interval have forms

$$c_B = 1.342 + 1.393\xi + 0.337\xi^2 - 0.747\xi^3 \quad (11)$$

in the first interval, and

$$c_B = -12.247 + 36.386\xi - 22.874\xi^2 \quad (12)$$

in the second interval.

Evidently, the desired value of the reactant output temperature in the output of the NPC can be computed for each c_B as

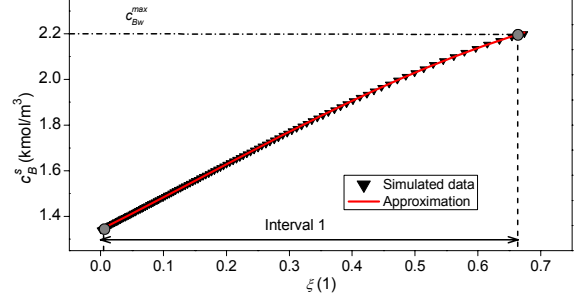


Figure 4: Steady-State Characteristics in the First Interval.

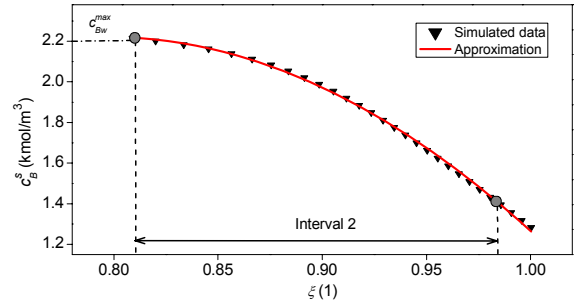


Figure 5: Steady-state Characteristics in the Second Interval.

$$\Delta T_{r,w} = G_w (T_{r,out}^{\max} - T_{r,out}^{\min}) \left(\frac{dc_B}{d\xi} \right)_{c_B}^{-1} \Delta c_{B,w} \quad (13)$$

where $\Delta c_{B,w} = c_{B,w} - c_B$ and G_w is a selectable gain coefficient.

The derivatives of approximate polynomials calculated from (11) and (12) take forms

$$\frac{dc_B}{d\xi} = 1.393 + 0.674\xi - 2.241\xi^2 \quad (14)$$

$$\frac{dc_B}{d\xi} = 36.386 - 45.748\xi \quad (15)$$

The derivatives of approximate polynomials can be seen in Figs. 6 and 7.

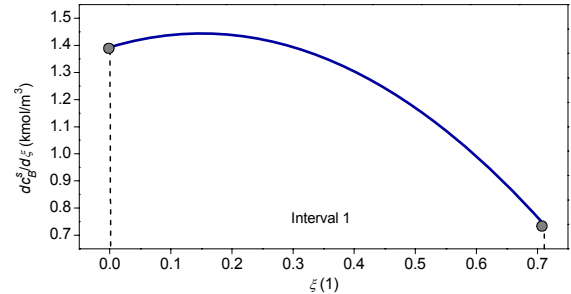


Figure 6: Approximate Polynomial Derivative in the First Interval.

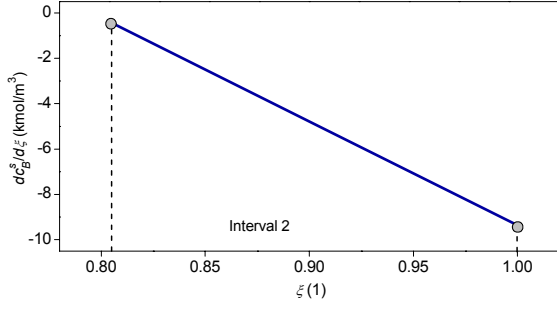


Figure 7: Approximate Polynomial Derivative in the Second Interval.

ADAPTIVE CONTROL SYSTEM DESIGN

Nonlinearity of the reactor is evident from the shape of the steady-state dependence of the output reactant temperature on the coolant flow rate shown in Fig. 8.

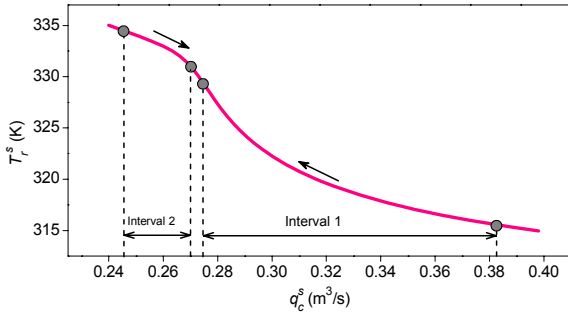


Figure 8: Dependence of the Output Reactant Temperature on the Coolant Flow Rate.

Note that all of the following control simulations are performed in intervals shown in Fig.8.

External Linear Model of the TCR

For the control purposes, the controlled output and the control input are defined as

$$u(t) = \Delta q_c(t) = q_c(t) - q_c^s \quad (16)$$

$$y(t) = \Delta T_{rout}(t) = T_{rout}(t) - T_{rout}^s \quad (17)$$

The CT ELM is proposed in the time domain on the basis of preliminary simulated step responses in the form of the second order differential equation

$$\ddot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_0 u(t) \quad (18)$$

and, in the complex domain, as the transfer function

$$G(s) = \frac{b_0}{s^2 + a_1 s + a_0} \quad (19)$$

External Delta Model

Establishing the δ operator

$$\delta = \frac{d-1}{T_0} \quad (20)$$

where δ is the forward shift operator and T_0 is the sampling period, the delta ELM corresponding to (18) takes the form

$$\delta^2 y(t') + a'_1 \delta y(t') + a'_0 y(t') = b'_0 u(t') \quad (21)$$

where t' is the discrete time.

When the sampling period is shortened, the delta operator approaches the derivative operator, and the estimated parameters a', b' reach the parameters a, b of the CT model.

Delta Model Parameter Estimation

Substituting $t' = k-2$, equation (21) can be rewritten to the form

$$\delta^2 y(k-2) + a'_1 \delta y(k-2) + a'_0 y(k-2) = b'_0 u(k-2). \quad (22)$$

Then, establishing the regression vector

$$\Phi_\delta^T(k-1) = (-\delta y(k-2) \quad -y(k-2) \quad u(k-2)) \quad (23)$$

where

$$\delta y(k-2) = \frac{y(k-1) - y(k-2)}{T_0} \quad (24)$$

the vector of delta model parameters

$$\Theta_\delta^T(k) = (a'_1 \quad a'_0 \quad b'_0) \quad (25)$$

is recursively estimated by the least squares method with exponential and directional forgetting from the ARX model (see, e.g. (Bobál et al. 2005) in the form

$$\delta^2 y(k-2) = \Theta_\delta^T(k) \Phi_\delta(k-1) + \varepsilon(k) \quad (26)$$

where

$$\delta^2 y(k-2) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_0^2}. \quad (27)$$

Adaptive Controller

The feedback control loop is depicted in Fig. 9. In the scheme, w is the reference signal, e denotes the tracking error, u the control input, and y the controlled output. The transfer function $G(s)$ of the CT ELM is given by (19). The reference w is considered as a step function.

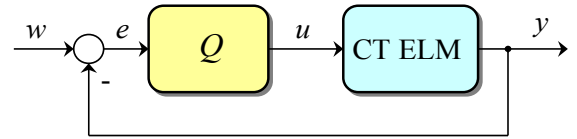


Figure 9: Feedback Control loop.

The feedback controller design is based on the polynomial approach. Procedure for designing can be briefly described as follows:

The transfer function of the controller is in the form

$$Q(s) = \frac{q(s)}{p(s)} \quad (28)$$

where q and p are coprime polynomials satisfying the condition of properness $\deg q(s) \leq \deg p(s)$.

As known, the problem is solved by controller whose polynomials are given by a solution of the polynomial equation

$$a(s)p(s) + b(s)q(s) = d(s) \quad (29)$$

with a stable polynomial $d(s)$ on the right side, with roots representing poles of the closed-loop, and where $p(s) = s\bar{p}(s)$ for step references.

In this paper, the polynomial $d(s)$ is considered in the form

$$d(s) = n(s)(s + \alpha)^2 \quad (30)$$

where the polynomial $n(s)$ is chosen as a result of spectral factorization

$$a^*(s)a(s) = n^*(s)n(s) \quad (31)$$

and α is a selectable double pole.

For $G(s)$ with $a(s) = s^2 + a_1s + a_0$, the resulting controller has the transfer function

$$Q(s) = \frac{q_2s^2 + q_1s + q_0}{s(s + p_0)} \quad (32)$$

with parameters computed from (26).

The above procedure implies that the controller parameters can be adjusted by the single selectable parameter α .

Simulation Experiments

Simulations document an effect of the concentration c_B measurement period and the adjustable part of the NPC gain on the control signals.

All simulations were performed on nonlinear model of the TCR. In the secondary control-loop, the P controller with a small gain was used at the start of simulations. For the δ -model parameter recursive identification, the sampling period $T_0 = 0.5$ s was chosen. The value of the selectable parameter α is stated under each figure.

In the first case, simulations in the first operating interval started from the point $c_B^s = 1.3504$ kmol/m³, $T_{rout}^s = 315.55$ K and $q_c^s = 0.383$ m³/s. The desired value of c_B has been chosen as $c_{Bw} = 2.2$ kmol/m³. An effect of the parameter G_w on the reference w , output temperature T_{rout} , the concentration c_B and the control input q_c responses is evident from Figs. 10 – 13.

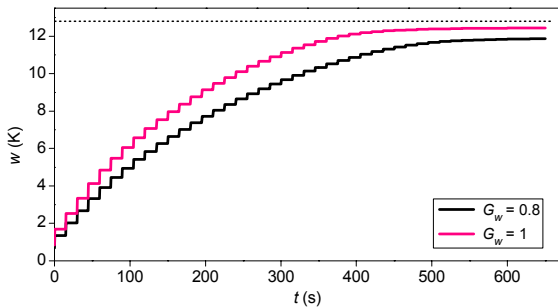


Figure 10: Reference Signal Courses ($t_s = 15$, $\alpha = 0.05$).

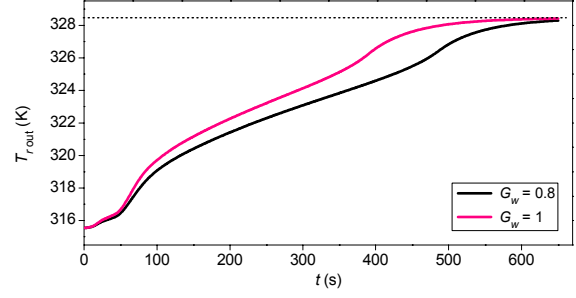


Figure 11: Reactant output temperature responses ($t_s = 15$, $\alpha = 0.05$).

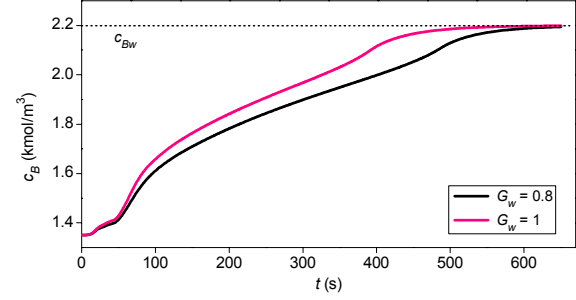


Figure 12: Concentration c_B responses ($t_s = 15$, $\alpha = 0.05$).

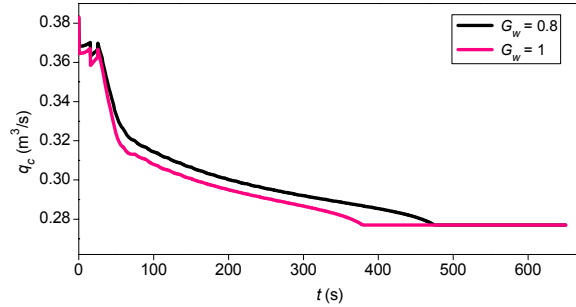


Figure 13: Coolant flow rate responses ($t_s = 15$, $\alpha = 0.05$).

It can be seen that an increasing G_w accelerates all signals in the control loop. However, its value is not unrestricted and its convenient value should be found experimentally.

An effect of the period t_s in the same operating interval can be seen in Figs.14 – 17. Although shortening t_s leads to faster control responses, its length is determined by possibilities of measurement.

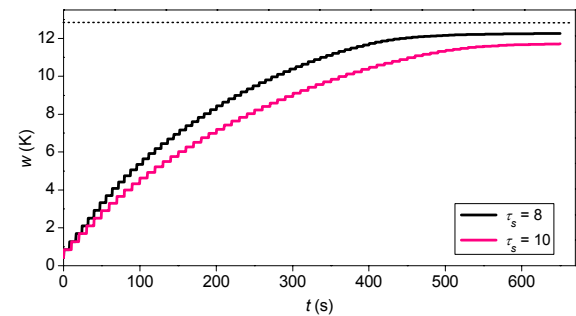


Figure 14: Reference Signal Courses ($G_w = 0.5$, $\alpha = 0.05$).

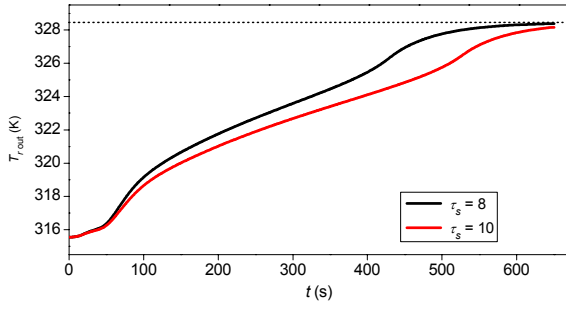


Figure 15: Reactant Output Temperature Responses ($G_w = 0.5$, $\alpha = 0.05$).

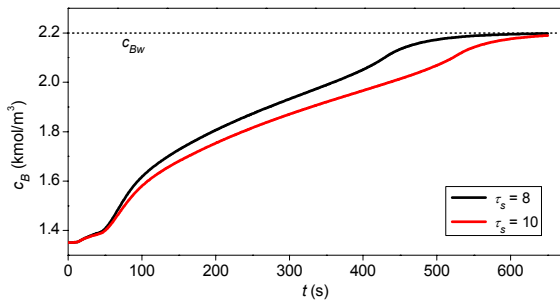


Figure 16: Concentration c_B responses ($G_w = 0.5$, $\alpha = 0.05$).

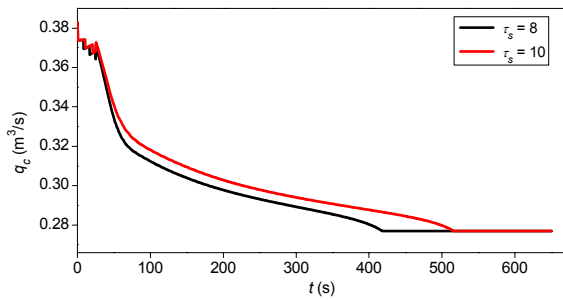


Figure 17: Coolant flow rate responses ($G_w = 0.$, $\alpha = 0.05$).

In the second case, simulations in the second operating interval started from the point $c_B^s = 1.3564$ kmol/m³, $T_{r,out}^s = 334.63$ K and $q_c^s = 0.244$ m³/s. The desired value of c_B has again been chosen as $c_{Bw} = 2.2$ kmol/m³. Here, only signal courses for $G_w = 1.2$, $t_s = 10$ and $\alpha = 0.08$ are presented. All signal courses are shown in Figs. 18 – 21.

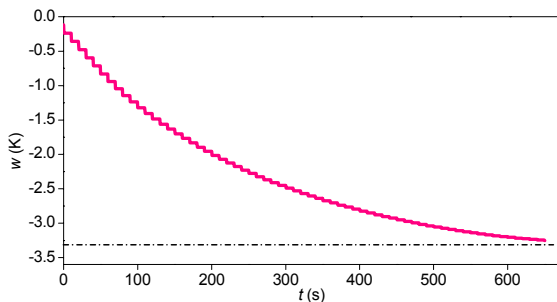


Figure 18: Reference Signal Course.

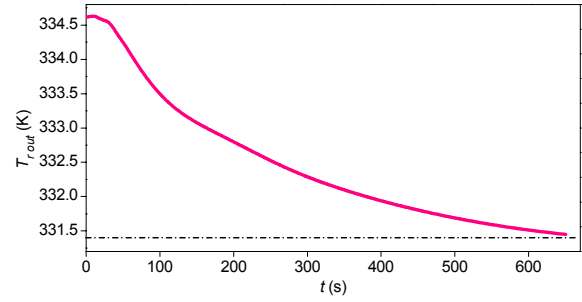


Figure 19: Reactant Output Temperature Response.

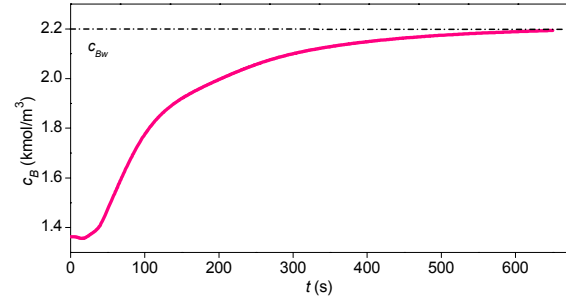


Figure 20: Concentration c_B response.

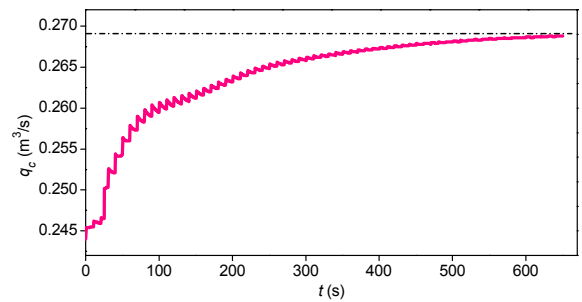


Figure 21: Coolant flow rate response.

CONCLUSIONS

The paper deals with design of the cascade control of a tubular chemical reactor. The presented procedure supposes measuring both the output concentration of a main reaction product and the output reactant temperature. The control is performed in the external and inner closed-loop where the concentration of a main product is the primary and an output reactant temperature the secondary controlled variable. A common control input is the coolant flow rate.

The controller in the external control-loop is a discrete nonlinear P-controller derived on the basis of simulated or measured steady-state characteristics of the reactor. The controller in the inner control-loop is an adaptive continuous-time controller. In its derivation, the recursive parameter estimation of an external delta model of the reactor, the polynomial approach and the pole placement method are applied.

The presented method has been tested by computer simulation on the nonlinear model of the tubular chemical reactor with a consecutive exothermic reaction.

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