Comparison of Two Approaches to Cascade Control of a CSTR

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Abstract**—**The paper deals with comparison of two approaches to cascade control of a continuous stirred tank chemical reactor. The control is performed in primary and secondary control-loops where the primary controlled output of the reactor is a concentration of the main reaction product. The secondary output is the reactant temperature. A common control input is the coolant flow rate. In the first case, the controller in the primary control-loop is a linear P-controller, and, in the second case a nonlinear P-controller. In both cases, the controller in the secondary control-loop is an adaptive controller. The results obtained on basis of both proposed approaches are verified by control simulations.

Keywords**—**chemical reactor, cascade control, external linear model, parameter estimation, adaptive control

I. Introduction

THE cascade control belongs to more complex control structures useful for such processes where more output variables can be measured and where only one input variable is available to the control. Principles of the cascade control are described e.g. in [1], [2], [3] and [4].

Chemical reactors are typical processes suitable for a use of the cascade control. In cases of non-isothermal reactions, concentrations of the reaction products mostly depend on the temperature of a 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 the cascade control design of a continuous stirred tank chemical reactor is presented.

Continuous stirred tank reactors (CSTRs) are units frequently used in chemical industry. From the system theory point of view, CSTRs belong to the class of nonlinear systems. Their mathematical models are described by sets of nonlinear differential equations (ODEs). The methods of CSTRs modelling and simulation can be found e.g. in [5], [6] and [7].

In this paper, the CSTR control strategy is based on the fact that concentrations of components of reactions taking place in the reactor depend on the reactant temperature. Then, the main product concentration is considered as the primary controlled variable, and, the reactant temperature as the secondary controlled variable. The coolant flow rate represents a common control input. Two types of primary controllers determining the set point for the secondary (inner) control-loop are considered. In the first case, the standard linear P-controller with an adjustable gain is used. In the second case, the nonlinear P-controller is designed on the basis of steady-state characteristics of the process. With respect to nonlinear dynamics of the reactor, the secondary adaptive controller is applied. On behalf of its development, the nonlinear model of the CSTR is approximated by a CT external linear model (ELM). For the CT ELM parameter estimation, the direct estimation in terms of filtered variables is used, see e.g. [8], [9] and [10]. The method is based on filtration of continuous-time input and output signals where the filtered variables have in the s-domain the same properties as their non-filtered counterparts. The resulting adaptive CT controller is derived on the basis of the polynomial approach and the pole placement method, see e.g. [11], [12] or [13]. Application of this method in the adaptive control is used e.g. in [14] – [17].

The control is tested by simulations of nonlinear model of the CSTR with a consecutive exothermic reaction.

II. Nonlinear Model of the CSTR

Consider a CSTR with exothermic reactions according to the scheme $A \xrightarrow{k_1} B$, $2B \xrightarrow{k_2} C$ and with a perfectly mixed cooling jacket. The desired product is the component *B*. Using usual simplifications, the model of the CSTR is described by four nonlinear differential equations

$$\frac{d c_A}{dt} = r_A + \frac{q_r}{V_r}(c_{Af} - c_A) \qquad (1)$$

$$\frac{d c_B}{dt} = r_B + \frac{q_r}{V_r}(c_{Bf} - c_B) \qquad (2)$$

$$\frac{dT_r}{dt} = \frac{h_r}{(\rho c_p)_r} + \frac{q_r}{V_r}(T_{rf} - T_r) + \frac{A_h U}{V_r(\rho c_p)_r}(T_c - T_r) \qquad (3)$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c}(T_{cf} - T_c) + \frac{A_h U}{V_c(\rho c_p)_c}(T_r - T_c) \qquad (4)$$

where

$$r_1 = k_1 c_A \quad r_2 = k_2 c_B^2 \qquad (5)$$

$$r_A = -r_1 \quad r_B = r_1 - r_2 \qquad (6)$$

and, with initial conditions $c_A(0) = c_A^s$, $c_B(0) = c_B^s$, $T_r(0) = T_r^s$ and $T_c(0) = T_c^s$. Here, *t* stands for the time, *c* for concentrations, *T* for temperatures, *V* for volumes, ρ for densities, c_p for specific heat capacities, *q* for volumetric flow rates, *r* for reaction rates, A_h is the heat exchange surface area and *U* is the heat transfer coefficient. Subscripts denoted *r* describe the reactant mixture, *c* the coolant, *f* the inlet values and the superscript *s* steady-state values.

The reaction rates and the reaction heat are expressed as

$$k_j = k_{0j} \exp\left(\frac{-E_j}{RT_r}\right),\ j = 1, 2 \qquad (7)$$

$$h_r = h_1 r_1 + h_2 r_2 \qquad (8)$$

where k_0 are pre-exponential factors, E are activation energies and h are reaction enthalpies. The values of all parameters, inlet values and their steady-state values are given in Table 1.

Table 1: Parameters and Inlet Values

V_r = 1.7 m^3 V_c = 0.64 m^3 ρ_r = 985 kg m^{-3} ρ_c = 998 kg m^{-3}	c_{pr} = 4.05 kJ kg^{-1}K^{-1} c_{pc} = 4.18 kJ kg^{-1}K^{-1} A_h = 5.65 m^2 U = 43.5 kJ m^{-2}min^{-1}K^{-1}
k_{10} = 5.616 · 10^{16} min^{-1} k_{20} = 1.128 · 10^{18} min^{-1} h_1 = 4.8 · 10^4 kJ kmol^{-1}	E_1/R = 13500 K E_2/R = 15400 K h_2 = 2.2 · 10^4 kJ kmol^{-1}
c_{Af}^s = 2.85 kmol m^{-3} T_{rf}^s = 323 K	c_{Bf}^s = 0 kmol m^{-3} T_{cf}^s = 293 K
q_r^s = 0.1 m^{3}min^{-1}	

III. The Control System Design

A basic scheme of the cascade control is in Fig. 1.

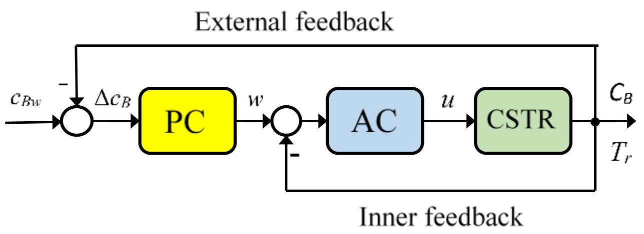

Fig. 1 Cascade nonlinear control scheme.

Here, PC stands for the primary linear (LPC) or nonlinear (NPC) proportional controller, AC for the secondary adaptive controller and CSTR for the reactor.

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 reactant temperature is in Fig. 2.

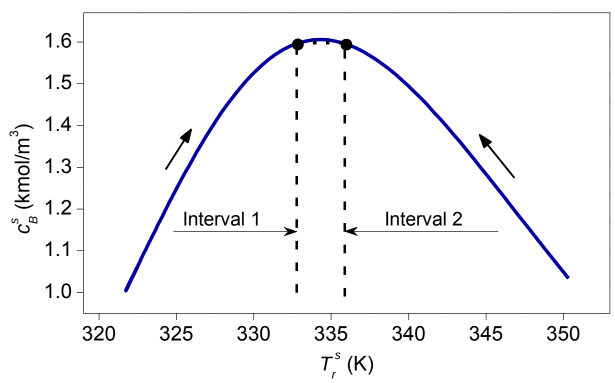

Fig. 2 Steady-state dependence of the product B concentration on the reactant temperature.

There, an operating area consists of two intervals. In the first interval, the concentration c_B increases with increasing reactant temperature, in the second interval it again decreases. Both intervals are limited to values

$$1.004 \le c_B \le 1.59, \quad 321.73 \le T_r \le 332.4$$

for the first interval, and,

$$1.59 \ge c_B \ge 1.034, \quad 336.15 \le T_r \le 350.33$$

for the second interval. In both intervals, the maximum value $c_B^{\max}$ = 1.59 kmol/m^2 is considered. It can be seen that the maximum value of c_B can be slightly higher then $c_B^{\max}$. However, with respect to some following procedures, the maximum desired value of c_B will be limited just by $c_B^{\max}$.

IV. The Primary Controllers

The primary P-controllers realize the relation between the deviation of desired and actual concentration c_B and the corresponding desired reaction temperature.

A. Linear P-controller

The LPC produces at each interval of measurement of c_B a desired reaction temperature according to the equation

$$\Delta T_{rw} = G_w \Delta c_{Bw} \qquad (9)$$

where G_w is an adjustable gain.

B. Nonlinear P-controller

The procedure in the design of the NPC appears from a gradual elaboration of computed or measured steady-state characteristics shown in Fig. 2.

In the first step, the temperature interval is transformed as

$$\xi = \frac{T_r - T_r^{\min}}{T_r^{\max} - T_r^{\min}}, \quad \xi \in \langle 0,1 \rangle \qquad (10)$$

where $T_r^{\min} = 321.73\,\mathrm{K}$, $T_r^{\max} = 350.3\,\mathrm{K}$.

The steady-state characteristics with transformed reactant temperature is shown in Fig. 3.

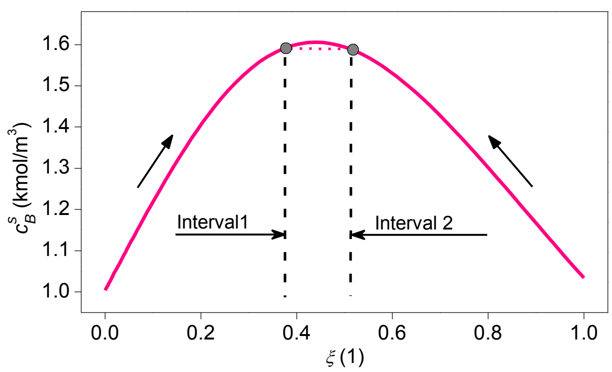

Fig 3 Steady-state dependence of component B concentration on transformed reactant tempereature.

In the next step, the inverse characteristics in both intervals are obtained changing axis in Fig. 3 as shown together with their approximations in Fig. 4. Then, characteristics in both intervals are approximated by polynomials in the form

$$\xi = 7.665 - 26.649 c_B + 33.823 c_B^2 - \\ -18.724 c_B^3 + 3.885 c_B^4 \qquad (11)$$

in the first interval, and,

$$\xi = 4.775 - 8.157 c_B + 6.061 c_B^2 - 1.643 c_B^3 \qquad (12)$$

in the second interval.

Derivatives of inverse steady-state characteristics according to (11) and (12) then are calculated as

$$\frac{d\xi}{dc_B} = -26.649 + 67.646c_B - 56.172c_B^2 + 15.54c_B^3 \quad (13)$$

in the first interval, and,

$$\frac{d\xi}{dc_B} = -8.157 + 12.122c_B - 4.922c_B^2 \quad (14)$$

in the second interval. The derivatives are shown in Fig. 5.

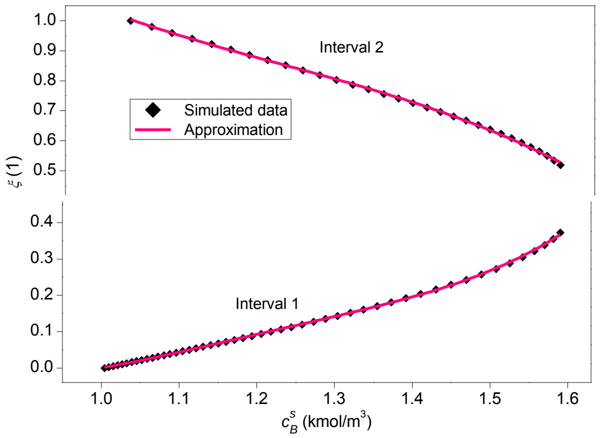

Fig. 4 Inverse steady state characteristics with approximation.

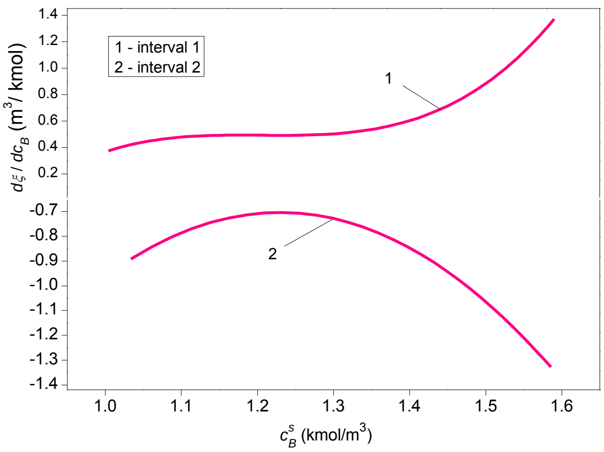

Fig. 5 Derivatives of inverse steady-state characteristics.

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

$$\Delta T_{rw} = K_w (T_{r\max} - T_{r\min}) \left(\frac{d\xi}{dc_B} \right)_{c_B} \Delta c_{Bw} \quad (15)$$

where $\Delta c_{Bw} = c_{Bw} - c_B^s$, $\Delta T_{rw} = T_{rw} - T_r^s$, and K_w is a selectable gain coefficient.

V. THE SECONDARY CONTROLLER DESIG

As previously introduced, the secondary controller is an adaptive linear controller. Nonlinearity of the reactor is evident from the shape of the steady-state dependence of the reactant temperature on the coolant flow rate shown in Fig. 6. Here, intervals for q_c corresponding to the above intervals for T_r are

$0.118 \le q_c \le 0.216$ in the first interval, and,

$0.04 \le q_c \le 0.1$ in the second interval.

Note that all of the following control simulations are performed in intervals shown in Fig.6.

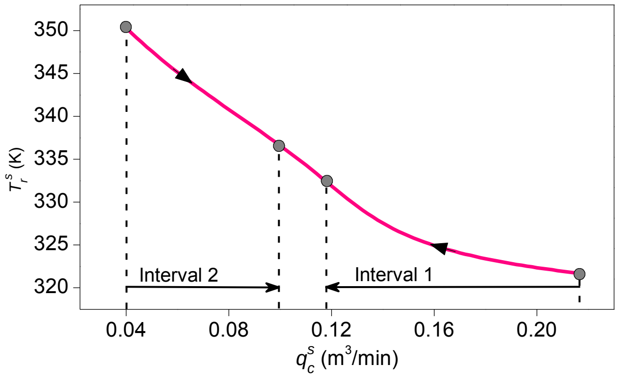

Fig. 6 Dependence of the reactant temperature on the coolant flow rate in the steady-state.

For the AC controller design, a continuous-time external linear model (CT ELM) of the CSTR with recursively estimated parameters is used. Further, the design procedure uses the polynomial approach with the pole assignment method.

A. CT external linear model of CSTR

The adaptive feedback control system is depicted in Fig. 7.

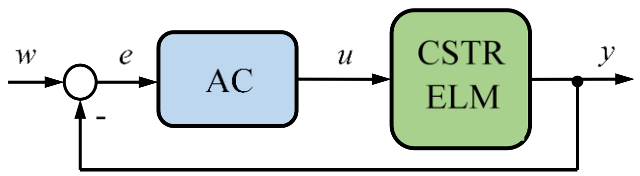

Fig. 7 Control system with CT external linear model.

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

$$u(t) = \Delta q_c(t) = q_c(t) - q_c^s \;,\; y(t) = \Delta T_r(t) = T_r(t) - T_r^s \quad (16)$$

and, $w = \Delta T_{rw}$.

The CT ELM is proposed in the time domain on the basis of not shown here preliminary simulated step responses in the form of the second order differential equation

$$\ddot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_0 u(t) \quad (17)$$

or, in the complex domain, as the transfer function

$$G(s) = \frac{b_0}{s^2 + a_1 s + a_0} \quad (18)$$

B. CT ELM parameter estimation

The method of the CT ELM parameter estimation can be briefly carried out as follows.

Since the derivatives of both input and output cannot be directly measured, filtered variables u_f and y_f are established as outputs of filters

$$c(\sigma) u_f(t) = u(t) \quad (19)$$

$$c(\sigma) y_f(t) = y(t) \quad (20)$$

where $\sigma = d/dt$ is the derivative operator, $c(\sigma)$ is a stable polynomial in σ that fulfills the condition $\deg c(\sigma) \geq \deg a(\sigma)$.

Note that the filter time constants must be smaller than the time constants of the process. Since the latter are unknown at the beginning of the estimation procedure, it is necessary to make the filter time constants, selected a priori, sufficiently small.

With regard to (17), the polynomial a takes the concrete form $a(\sigma) = \sigma^2 + a_1\sigma + a_0$, and, the polynomial c can be chosen as $c(\sigma) = \sigma^2 + c_1\sigma + c_0$. Subsequently, the values of the filtered variables can be computed during the control by a solution of (19) and (20) using some standard integration method.

It can be easily proved that the transfer behavior among filtered and among unfiltered variables are equivalent.

Filtered variables including their derivatives can be sampled from filters (19) and (20) in discrete time intervals $t_k = k\, T_S$, $k = 0,1,2, ...$ where T_S is the sampling period. Now, the regression vector is defined as

$$\boldsymbol{\Phi}(t_k) = \left(-y_f(t_k) \ \ -\dot{y}_f(t_k) \ \ u_f(t_k) \ \ 1\right) \tag{21}$$

and, the vector of parameters

$$\boldsymbol{\Theta}^T(t_k) = \left(a_0 \ \ a_1 \ \ b_0\right) \tag{22}$$

can be estimated from the ARX model

$$\ddot{y}_f(t_k) = \boldsymbol{\Theta}^T(t_k)\boldsymbol{\Phi}(t_k) + e(t_k) \tag{23}$$

Here, the recursive identification method with exponential and directional forgetting was used according to [18].

C. Adaptive Controller

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

The transfer function of the AC controller in Fig. 7 is

$$Q(s) = \frac{q(s)}{p(s)} \tag{24}$$

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

The reference w is considered as a sequence of step functions with transform

$$W_k(s) = \frac{w_{k0}}{s}. \tag{25}$$

In this paper, the disturbance is not considered.

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

$$a(s)p(s) + b(s)q(s) = d(s) \tag{26}$$

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

For deg $a = 2$, the controller transfer function (24) takes the form

$$Q(s) = \frac{q(s)}{s\,\tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s(s + p_0)} \tag{27}$$

The controller parameters then follow from solution of the polynomial equation (26) and depend upon coefficients of the polynomial d.

In this paper, the polynomial d with roots determining the closed-loop poles is chosen as

$$d(s) = n(s)(s + \alpha)^2 \tag{28}$$

where n is a stable polynomial obtained by spectral factorization

$$a^*(s)a(s) = n^*(s)n(s) \tag{29}$$

and α is the selectable parameter that can usually be chosen by way of simulation experiments. Note that a choice of d in the form (28) provides the control of a good quality for aperiodic controlled processes. The polynomial n has the form $n(s) = s^2 + n_1 s + n_0$ with coefficients

$$n_0 = \sqrt{a_0^2}\ , \quad n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0}\ . \tag{30}$$

The controller parameters can be obtained from solution of the matrix equation

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ a_1 & b_0 & 0 & 0 \\ a_0 & 0 & b_0 & 0 \\ 0 & 0 & 0 & b_0 \end{pmatrix} \times \begin{pmatrix} p_0 \\ q_2 \\ q_1 \\ q_0 \end{pmatrix} = \begin{pmatrix} d_3 - a_1 \\ d_2 - a_0 \\ d_1 \\ d_0 \end{pmatrix} \tag{31}$$

where

$$\begin{gathered} d_3 = n_1 + 2\alpha,\ d_2 = 2\alpha n_1 + n_0 + \alpha^2 \\ d_1 = 2\alpha n_0 + \alpha^2 n_1,\ d_0 = \alpha^2 n_0 \end{gathered}. \tag{32}$$

Evidently, the controller parameters can be adjusted by the selectable parameter α.

VI. Simulation Results

All simulations were performed on nonlinear model of the CSTR. Concentrations c_B are measured in periods t_s (min). The aim of simulations is to compare control responses obtained by using linear and nonlinear primary controller.

The some gains of both controllers were calculated at start of all simulations. For the direct recursive parameter estimation, the sampling period T_S = 1 min was chosen. The value of the selectable closed-loop pole α = 0.1 has been chosen in all simulations. Values of other parameters are listed below figures.

All simulations in the first operating interval started from the point $c_B^s = 1.11\,\text{kmol/m}^3$, $T_r^s = 323.05\,\text{K}$ and $q_c^s = 0.186$ m^3/min. The desired value of c_B has been chosen as $c_{Bw} = 1.58$ kmol/m^3. The simulation results are shovn in Figs. 8 – 14.

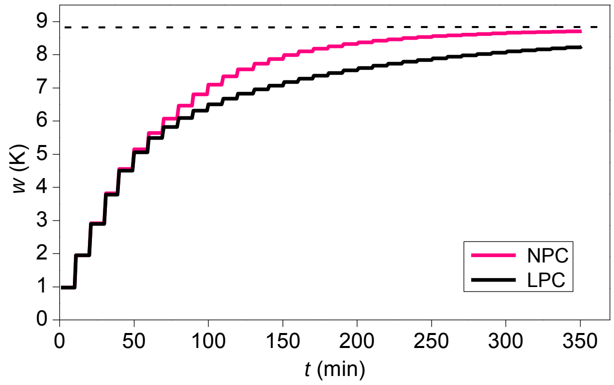

Fig. 8 Reference signal courses ($K_w = 0.15$, $G_w = 2.05$, $t_s = 10$).

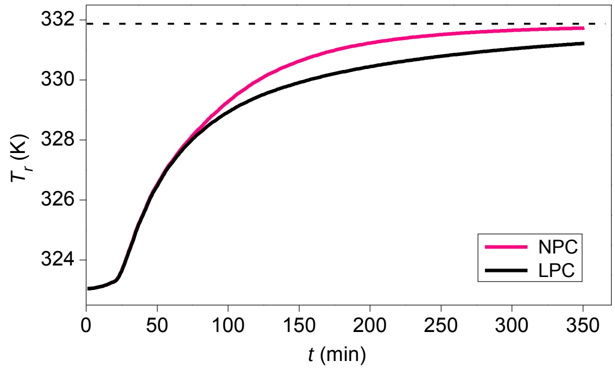

Fig. 9 Reactant temperature responses ($K_w = 0.15$, $G_w = 2.05$, $t_s = 10$).

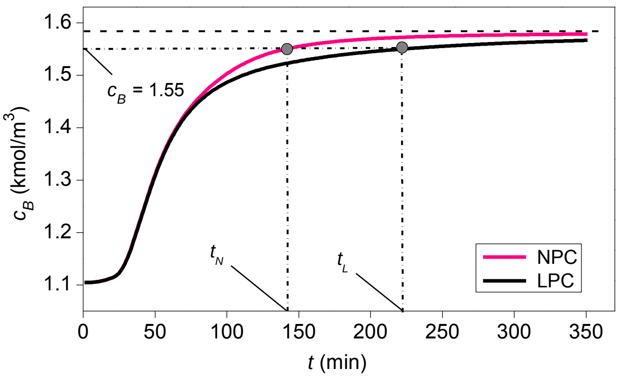

Fig. 10 Concentration c_B responses ($K_w = 0.15$, $G_w = 2.05$, $t_s = 10$).

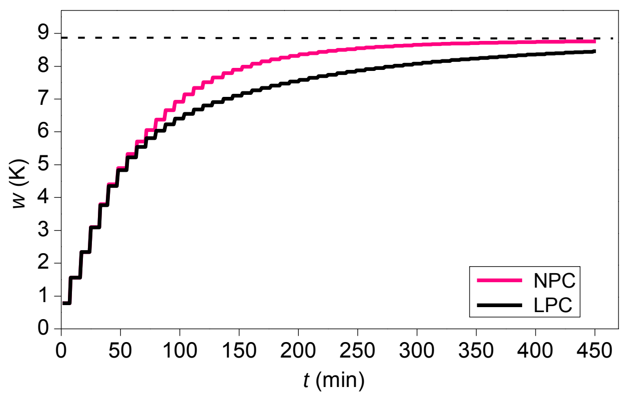

Fig. 11 Reference signal courses ($K_w = 0.12$, $G_w = 1.645$, $t_s = 8$).

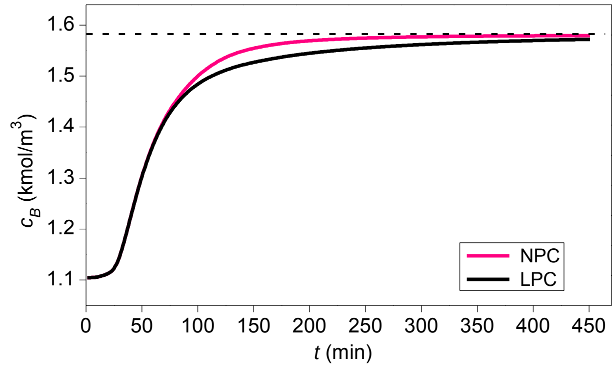

Fig. 12 Concentration c_B responses ($K_w = 0.12$, $G_w = 1.645$, $t_s = 8$).

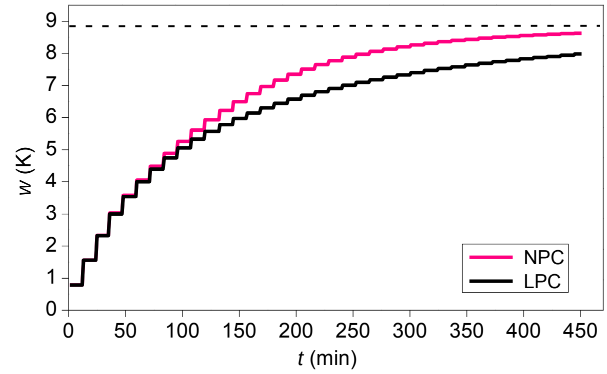

Fig. 13 Reference signal courses ($K_w = 0.12$, $G_w = 1.645$, $t_s = 12$).

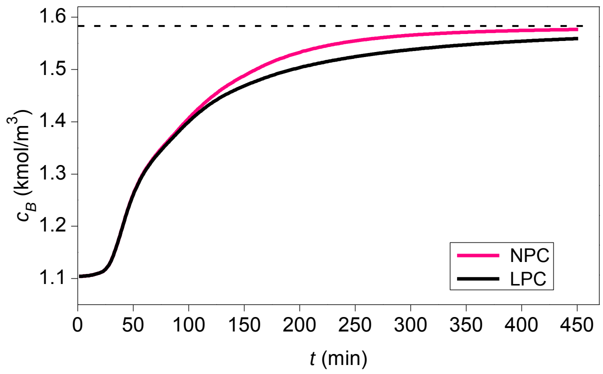

Fig. 14 Concentration c_B responses ($K_w = 0.12$, $G_w = 1.645$, $t_s = 12$).

It can be seen that a use of the NPC leads to faster signal courses. For example, the value $c_B = 1.55$ kmol/m^3 is reached by the NPC in $t_N = 142$ min, but by LPC in $t_L = 222$ min, as shown in Fig. 10. This fact is given by increasing trend of the derivative $\left(\dfrac{d\xi}{d c_B}\right)$ in the first interval, see, Fig. 5.

Simulations in the second operating interval started from the point $c_B^s = 1.11\,\text{kmol/m}^3$, $T_r^s = 348.63\,\text{K}$ and $q_c^s = 0.046$ m^3/min. The desired value of c_B has been again chosen as $c_{Bw} = 1.58$ kmol/m^3. The simulation results are shovn in Figs. 15 – 17.

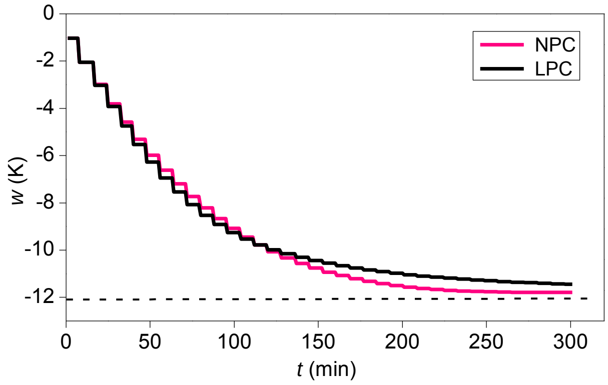

Fig. 15 Reference signal courses (K_w = 0.1, G_w = - 2.206, t_s = 8).

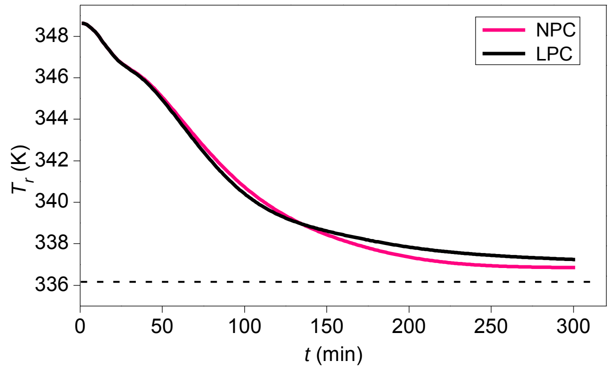

Fig. 16 Reactant temperature responses (K_w = 0.1, G_w = - 2.206, t_s = 8).

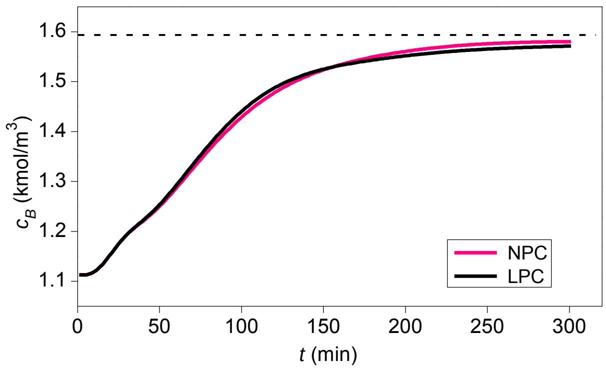

Fig. 17 Concentration c_B responses (K_w = 0.1, G_w = - 2.206, t_s = 8).

Here, a difference between LPC and NPC is not significant. This fact is again determined by the shape of the inverse characteristics derivative in the second interval as shown in Fig. 5.

For interest, the time course of the coolant flow rate is shown in Fig. 18.

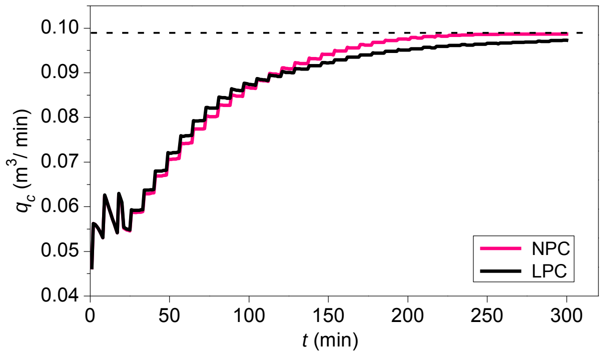

Fig. 18 Coolant flow rate courses (K_w = 0.1, G_w = - 2.206, t_s = 8).

VII. Conclusions

The article presents a comparison of two ways to the cascade control of a continuous stirred tank reactor. In both cases, the control is performed in the external (primary) and inner (secondary) closed-loop where the concentration of a main product is the primary and the reactant temperature the secondary controlled variable. A common control input is the coolant flow rate.

In the first case, the controller in the external control-loop is a linear P-controller with an adjustable gain. In the second case, this gain of the nonlinear P-controller depends on the derivative of an inverse steady-state characteristics. The controller in the inner control-loop is an adaptive controller which of derivation the recursive parameter estimation, the polynomial approach and the pole placement method were applied.

The control was tested by simulations on the nonlinear model of the CSTR.

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