SIMULATION OF CASCADE CONTROL OF A CONTINUOUS STIRRED TANK REACTOR

Petr Dostál^{1,2}, Vladimír Bobál^{1,2}, and Jiří Vojtěšek² ¹Centre of Polymer Systems, University Institute, Tomas Bata University in Zlin, Nad Ovcirnou 3685, 760 01 Zlin, Czech Republic. ² Department of Process Control, Faculty of Applied Informatics, Tomas Bata University in Zlin, Nad Stranemi 4511, 760 05 Zlin, Czech Republic {dostalp;bobal;vojtesek}@fai.utb.cz

KEYWORDS

Adaptive control, cascade control, continuous stirred tank reactor, control simulation.

ABSTRACT

The paper presents simulation results of the cascade control of a continuous stirred tank reactor. The control is performed in primary and secondary control-loops where the primary controlled output of the reactor is the concentration of a desired reaction product, and, the secondary output is the reactant temperature. A common control input is the coolant flow rate. The controller in the primary control-loop is a P-controller with the gain calculated using simulated or measured steady-state characteristics of the reactor. The controller in the secondary control-loop is an adaptive controller. The proposed method is verified by control simulations

INTRODUCTION

The cascade control method allows the control of processes with a main and secondary controlled variable and with a single control input. The method is especially useful when a main controlled output can be measured only in longer time intervals and with an additional output measurable in shorter time periods. Principles of the cascade control are described e.g. in (Bequette 2006; Mahoney et al. 2006; Seborg et al. 1989; Smuts 2011).

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 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 cascade control description of a continuous stirred tank reactor (CSTR) with results of control simulations is presented.

CSTRs are apparatus widely used in chemical industry, biotechnologies, polymer manufacturing, and many others. From the system theory point of view, CSTRs belong to a class of nonlinear systems with mathematical models described by sets of nonlinear differential equations as it can be seen e.g. in (Smith 2005; Corriou 2004).

Here, in the cascade control-loop, the concentration of a desired product of reactions is considered as the primary

Proceedings 29th European Conference on Modelling and Simulation ©ECMS Valeri M. Mladenov, Petia Georgieva, Grisha Spasov, Galidiya Petrova (Editors) ISBN: 978-0-9932440-0-1 / ISBN: 978-0-9932440-1-8 (CD) controlled variable, and, the reactant temperature as the secondary controlled variable. The coolant flow rate represents a common control input.

The primary control variable is measured in discrete time intervals. The primary controller determining the set point for the secondary (inner) control-loop is a discrete nonlinear proportional controller derived on the basis of steady-state characteristics of the reactor. 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 the nonlinear model of the CSTR by a continuous-time external linear model (CT ELM) with recursively estimated parameters. In the process of parameter estimation, the direct method by (Rao and Unbehauen 2006); Garnier and Wang 2008) is used. The control loop with two feedback adaptive controllers is used, see, e.g. (Dostál et al. 2007). The resulting controllers are derived by the pole placement method, see, e.g. (Grimble 1993; Kučera 1993; Brogan 1991; Franklin et al. 2006).

The cascade control is verified by simulations on the nonlinear model of the CSTR.

NONLINEAR MODEL OF THE CSTR

Consider a CSTR with exothermic reactions according to the scheme $A \rightarrow B$, $2B \rightarrow C$ 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

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

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

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

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

where

$$r_1 = k_1 c_A \quad r_2 = k_2 c_B^2 \tag{5}$$

$$r_A = -r_1 \quad r_B = r_1 - r_2$$
 (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

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

$$h_r = h_1 r_1 + h_2 r_2 \tag{8}$$

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.

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

Table 1: Parameters and Inlet Values

THE CONTROL OBJECTIVE

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



Figure 1: Cascade control scheme.

Here, PC stands for the nonlinear proportional controller, AC for the 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.

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. Simulation of the steady-state characteristics was performed in the interval $320 \text{ K} \le T_r \le 355 \text{ K}$. The product *B* concentration reaches a maximum value higher than 1.6 kmol/m³. However, with respect to some following procedures, the maximum desired value c_B will be limited just by $c_{Bw}^{\text{max}} = 1.6 \text{ kmol/m}^3$.



Figure 2: Steady-state dependence of the product *B* concentration on the reactant temperature.

THE PC DESIGN

The procedure in the design of the nonlinear PC appears from polynomial approximation of the steady-state characteristics.

The boundaries of operating intervals are determined as

 $0.873 \le c_B \le 1.6$, $320 \le T_r \le 333.5$

in the first operating interval, and

$$1.6 \ge c_B \ge 0.833$$
, $335.5 \le T_r \le 355$

in the second operating interval.

For purposes of approximation, the temperature is transformed as

$$\xi = \frac{T_r - T_r^{\min}}{T_r^{\max} - T_r^{\min}}, \quad \xi \in \langle 0, 1 \rangle \tag{9}$$

where $T_r^{\min} = 320 \,\text{K}$, $T_r^{\max} = 355 \,\text{K}$.

The steady-state characteristics with transformed reactant temperature can be seen in Fig. 3.



Figure 3: Steady-state dependence of the product *B* concentration on transformed reactant temperature.

Further, the polynomial approximations of steady-state characteristics in above intervals including their

derivatives take forms

$$c_B^s = -7.1282\xi^3 + 0.6968\xi^2 + 2.6767\xi + 0.8718$$
(10)

$$\frac{dc_B^3}{d\xi} = -21.3846\xi^2 + 1.3936\xi + 2.6767$$
(11)

in the first operating interval, and,

$$c_B^s = 3.3209\xi^3 - 7.8785\xi^2 + 4.5473\xi + 0.847 \quad (12)$$

$$\frac{dc_B^3}{d\xi} = 9.9627\xi^2 - 15.757\xi + 4.5473 \tag{13}$$

in the second operating interval.

Steady-state characteristics in both intervals together with their approximations are in Figs. 4 and 5.



Figure 4: Steady-state characteristics in the interval 1.



Figure 5: Steady-state characteristics in the interval 2.

Now, a difference of the desired value of the reactant temperature in the output of the PC can be computed for each c_B as

$$\Delta T_{rw} = G_w (T_r^U - T_r^L) \left(\frac{d\xi}{dc_B} \right)_{c_B} \Delta c_{Bw}$$
(14)

where G_w is a selectable gain coefficient.

The derivative in (14) is calculated from inversion of (11) and (13).

ADAPTIVE CONTROLLER DESIGN

The steady-state dependence of the reactant temperature on the coolant flow rate can be seen in Fig. 6. Its nonlinearity is evident. It should be noted that the desired temperature value shall not be from the interval $333.5 < T_r < 335.5$. This requirement can be fulfilled by programming means.

External Linear Model of the CSTR

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



Figure 6: Steady-state dependence of reactant temperature on the coolant flow rate.

$$y(t) = \Delta T_r(t) = T_r(t) - T_r^s$$
, $u(t) = q_c(t) - q_c^s$. (15)

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

$$\ddot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_0 u(t)$$
 (16)

and, in the complex domain as the transfer function

$$G(s) = \frac{b_0}{s^2 + a_1 s + a_0}.$$
 (17)

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

$$c(\sigma)u_f(t) = u(t) \tag{18}$$

$$c(\sigma)y_f(t) = y(t) \tag{19}$$

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

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 (18) and (19) 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 (18) and (19) 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

$$\boldsymbol{\Phi}(t_k) = \left(-y_f(t_k) - \dot{y}_f(t_k) u_f(t_k) 1\right)$$
(20)

and, the vector of parameters

$$\boldsymbol{\Theta}^{T}(t_{k}) = \begin{pmatrix} a_{0} & a_{1} & b_{0} \end{pmatrix}$$
(21)

can be estimated from the ARX model

$$\ddot{y}_f(t_k) = \boldsymbol{\Theta}^T(t_k) \boldsymbol{\Phi}(t_k) + \boldsymbol{e}(t_k) \,. \tag{22}$$

Here, the recursive identification method with exponential and directional forgetting was used according to (Bobál et al. 2005).

Controller Design

The control system with two feedback controllers is depicted in Fig.7.



Figure 7: Control System.

In the scheme, w is the reference signal $w = T_{rw} - T_r^s$, y denotes the controlled output, e the tracking error and u the controller output. The sequence of reference signals is composed of step functions with the transform

$$W_k(s) = \frac{w_{0k}}{s}.$$
 (23)

The transfer function G represents approximate transfer function in the general form (17).

The transfer functions of controllers are

$$Q(s) = \frac{\tilde{q}(s)}{\tilde{p}(s)}, \quad R(s) = \frac{r(s)}{\tilde{p}(s)}$$
(24)

where \tilde{q} , *r* and \tilde{p} are coprime polynomials in *s*.

The design of controllers described in this section follows from the polynomial approach. The derivation is described in detail e.g. in (Dostál et al. 2012).

The result of derivation can be summarized as follows: The polynomials in (24) are given by a solution of the polynomial equation

$$d(s) = a(s)\tilde{p}(s) + b(s)(r(s) + \tilde{q}(s))$$
(25)

where d is a characteristic polynomial with roots as poles of the closed-loop.

Establishing the polynomial *t* as

$$t(s) = r(s) + \tilde{q}(s) \tag{26}$$

and substituting (26) into (25), the polynomials \tilde{p} and t are given by a solution of the polynomial equation

$$a(s)\tilde{p}(s) + b(s)t(s) = d(s)$$
(27)

with a stable polynomial *d* on the right side.

With regard to the transforms (23), the asymptotic tracking is provided for polynomials \tilde{p} and \tilde{q} having forms

$$\tilde{p}(s) = s \, p(s) \,, \quad \tilde{q}(s) = s \, q(s) \,.$$
 (28)

Subsequently, the transfer functions (24) take forms

$$Q(s) = \frac{q(s)}{p(s)}, \quad R(s) = \frac{r(s)}{sp(s)}$$
 (29)

It can be easily proved that the degrees of polynomials q and r must fulfil inequalities

$$\deg q \le \deg p , \ \deg r \le \deg p + 1.$$
 (30)

Now, the polynomial t can be rewritten to the form

$$t(s) = r(s) + s q(s)$$
. (31)

Subsequently, the degrees of polynomials in (27) and (29) can be easily derived as

$$\deg t = \deg r = \deg a, \ \deg q = \deg a - 1 \deg p \ge \deg a - 1, \ \deg d \ge 2 \deg a$$
 (32)

Then, denoting deg a = n, polynomials t, r and q have forms

$$t(s) = \sum_{i=0}^{n} t_i s^i , \ r(s) = \sum_{i=0}^{n} r_i s^i , \ q(s) = \sum_{i=1}^{n} q_i s^{i-1}$$
(33)

and, relations among their coefficients are

$$r_0 = t_0, \quad r_i + q_i = t_i \text{ for } i = 1, \dots, n.$$
 (34)

Since by a solution of the polynomial equation (27) provides calculation of coefficients t_i , unknown coefficients r_i and q_i can be obtained by a choice of selectable coefficients $\beta_i \in \langle 0, 1 \rangle$ such that

$$r_i = \beta_i t_i, \quad q_i = (1 - \beta_i) t_i \text{ for } i = 1, ..., n.$$
 (35)

The coefficients β_i distribute a weight between numerators of transfer functions *Q* and *R*.

For the second order model (17) with deg a = 2, the controller's transfer functions take specific forms

$$Q(s) = \frac{q(s)}{p(s)} = \frac{q_2 s + q_1}{s + p_0}$$

$$R(s) = \frac{r(s)}{s p(s)} = \frac{r_2 s^2 + r_1 s + r_0}{s (s + p_0)}$$
(36)

where

$$r_0 = t_0, r_1 = \beta_1 t_1, r_2 = \beta_2 t_2$$

$$q_1 = (1 - \beta_1) t_1, q_2 = (1 - \beta_2) t_2.$$
(37)

The controller parameters then result from a solution of the polynomial equation (27) and depend upon coefficients of the polynomial d. The next problem here is to find a stable polynomial d that enables to obtain acceptable stabilizing controllers.

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

$$d(s) = n(s)(s+\alpha)^2$$
(38)

where n is a stable polynomial obtained by spectral factorization

$$a^*(s)a(s) = n^*(s)n(s)$$
 (39)

and α is the selectable parameter.

The coefficients of n then are expressed as

$$n_0 = \sqrt{a_0^2}$$
, $n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0}$ (40)

and, the controller parameters p_0 and t can be obtained from solution of the matrix equation

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ a_1 & b_0 & 0 & 0 \\ a_0 & 0 & b_0 & 0 \\ 0 & 0 & 0 & b_0 \end{pmatrix} \times \begin{pmatrix} p_0 \\ t_2 \\ t_1 \\ t_0 \end{pmatrix} = \begin{pmatrix} d_3 - a_1 \\ d_2 - a_0 \\ d_1 \\ d_0 \end{pmatrix}$$
(41)

where

$$d_{3} = n_{1} + 2\alpha, d_{2} = 2\alpha n_{1} + n_{0} + \alpha^{2}$$

$$d_{1} = 2\alpha n_{0} + \alpha^{2} n_{1}, d_{0} = \alpha^{2} n_{0}$$
(42)

Now, it follows from the above introduced procedure that tuning of controllers can be performed by a suitable choice of selectable parameters β and α .

The controller parameters r and q can then be obtained from (37).

SIMULATION RESULTS

The goal of simulations is to show the effect of selectable parameters on the control courses. In this paper, the control simulations were performed only in the first operating interval.

The simulations started at the starting point $c_A^s = 1.6677 \text{ kmol/m}^3$, $c_B^s = 1.1311 \text{ kmol/m}^3$, $T_r^s = 323.4 \text{ K}$, $T_c^s = 300.5 \text{ K}$ and $q_c^s = 0.18 \text{ m}^3/\text{min}$. In all simulations, the desired value $c_{Bw} = 1.6 \text{ kmol/m}^3$ has been chosen. For the start (the adaptation phase), the P controller with a small gain was used in all simulations.

An effect of the parameter G_w on the control is evident from Figs. 8 – 10. 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. 11 – 13. Although shortening t_s leads to faster control responses, its length is determined by measurement possibilities. The tendency to overshoots at small measurement periods can be suppressed by selecting a lower gain G_w .

An influence of the closed- loop pole α on the control responses can be seen in Figs. 14 – 16. Choosing a higher α values can lead to oscillations.

The last group of simulations in Figs. 17 - 19 shows an influence of the parameter β_2 on the control courses. Here were chosen only by his extreme values. It can be seen that in an favorable choice of other parameters, the

control quality can be improved just by a suitable option of parameters β .



Figure 8: Effect of G_w : Reference Signal Courses $(t_s = 10, \alpha = 0.1, \beta_1 = \beta_2 = 1).$



Figure 9: Effect of G_w : Reactant Temperature Responses ($t_s = 10$, $\alpha = 0.1$, $\beta_1 = \beta_2 = 1$).



Figure 10: Effect of G_w : Concentration Responses $(t_s = 10, \alpha = 0.1, \beta_1 = \beta_2 = 1).$



Figure 11: Effect of t_s : Reference Signal Courses $(G_w = 0.1, \alpha = 0.1, \beta_1 = \beta_2 = 1).$



Figure 12: Effect of t_s : Reactant Temperature Responses ($G_w = 0.1$, $\alpha = 0.1$, $\beta_1 = \beta_2 = 1$).



Figure 13: Effect of t_s : Concentration Responses $(G_w = 0.1, \alpha = 0.1, \beta_1 = \beta_2 = 1).$



Figure 14: Effect of α : Reference Signal Courses $(G_w = 0.15, t_s = 10, \beta_1 = \beta_2 = 1).$







Figure 17: Effect of β : Reference Signal Courses $(G_w = 0.15, t_s = 10, \alpha = 0.15).$



Figure 18: Effect of β : Reactant Temperature Responses ($G_w = 0.15$, $t_s = 10$, $\alpha = 0.15$).



CONCLUSIONS

The paper deals with the cascade control of a continuous stirred tank reactor. A necessary condition for a use of the presented method is measurement of a main product of the reaction taking place in the reactor. The control is performed in the external and inner 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.

The controller in the external control-loop is a discrete nonlinear P-controller derived on the basis of steadystate characteristics of the reactor. The inner controlloop consists of two adaptive feedback controllers. For their derivation, the recursive parameter estimation, the polynomial approach and the pole placement method are applied.

The paper contains numerous simulations documenting the influence of each selectable controller parameters on the control.

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AUTHOR BIOGRAPHIES

PETR DOSTÁL studied at the Technical University of Pardubice, Czech Republic, where he obtained his master degree in 1968 and PhD. degree in Technical Cybernetics in 1979. In the year 2000 he became professor in Process Control. He is now head of the Department of Process Control, Faculty of Applied Informatics of the Tomas Bata University in Zlín. His research interests are modelling and simulation of continuous-time chemical processes, polynomial methods, optimal and adaptive control. You can contact him on email address <u>dostalp@fai.utb.cz</u>.

VLADIMÍR BOBÁL graduated in 1966 from the Brno University of Technology, Czech Republic. He received his Ph.D. degree in Technical Cybernetics at Institute of Technical Cybernetics, Slovak Academy of Sciences, Bratislava, Slovak Republic. He is now Professor at the Department of Process Control, Faculty of Applied Informatics of the Tomas Bata University in Zlín, Czech Republic. His research interests are adaptive and predictive control, system identification, time-delay systems and CAD for automatic control systems. You can contact him on email address <u>bobal@fai.utb.cz</u>

JIŘÍ VOJTĚŠEK studied at Tomas Bata University in Zlin, Czech Republic, where he received his M.Sc. degree in Automation and control in 2002. In 2007 he obtained Ph.D. degree in Technical cybernetics at Tomas Bata University in Zlin. He now works as an assistant professor at the Department of Process Control, Faculty of Applied Informatics of the Tomas Bata University in Zlin, Czech Republic. His research interests are modeling and simulation of continuoustime chemical processes, polynomial methods, optimal, adaptive and nonlinear control.

You can contact him on email address vojtesek@fai.utb.cz