Slovak University of Technology in Bratislava
Institute of Information Engineering, Automation, and Mathematics

PROCEEDINGS

of the 18$^{\text{th}}$ International Conference on Process Control

Hotel Titris, Tatranská Lomnica, Slovakia, June 14 – 17, 2011

ISBN 978-80-227-3517-9

http://www.kirp.chtf.stuba.sk/pc11

Editors: M. Fikar and M. Kvasnica

Dostál, P., Bobál, V., Vojtěšek, J.: Nonlinear Control of a Chemical Reactor, Editors: Fikar, M., Kvasnica, M., In *Proceedings of the 18th International Conference on Process Control*, Tatranská Lomnica, Slovakia, 38–43, 2011.

Full paper online: http://www.kirp.chtf.stuba.sk/pc11/data/abstracts/014.html

Nonlinear Control of a Chemical Reactor

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Abstract: The paper deals with continuous-time nonlinear adaptive control of a continuous stirred tank reactor. The control strategy is based on an application of the controller consisting of a linear and nonlinear part. The static nonlinear part is derived in the way of a inversion and consecutive polynomial approximation of a measured or simulated input-output data. The design of the dynamic linear part is based on approximation of nonlinear elements in the control loop by a continuous-time external linear model with parameters estimated using a corresponding delta model. In the control design procedure, the polynomial approach with the pole assignment method is used. The nonlinear adaptive control is tested by simulations on the nonlinear model of the CSTR with a consecutive exothermic reaction.

1. INTRODUCTION

Continuous stirred tank reactors (CSTRs) are units frequently used in chemical and biochemical industry. From the system theory point of view, CSTRs belong to a class of nonlinear systems. Their mathematical models are described by sets of nonlinear differential equations. Their models are derived and described in e.g. Ogunnaike and Ray (1994), Schmidt (2005) and Corriou (2004).

It is well known that the control of chemical reactors often represents very complex problem. The control problems are due to the process nonlinearity and high sensitivity of the state and output variables to input changes. In addition, the dynamic characteristics may exhibit a varying sign of the gain in various operating points as well as non-minimum phase behaviour. Evidently, the process with such properties is hardly controllable by conventional control methods, and, its effective control requires application some of advanced methods.

One possible method to cope with this problem exploits a linear adaptive controller with parameters computed and readjusted on the basis of recursively estimated parameters of an appropriate chosen continuous-time external linear model (CT ELM) of the process. Some results obtained by this method can be found in e.g. Dostál et al. (2007) and Dostál et al. (2009).

An effective approach to the control of CSTRs and similar processes utilizes various methods of the nonlinear control (NC). Several modifications of the NC theory are described in e.g. Astolfi et al. (2008), Vincent and Grantham (1997), Ioannou and Fidan (2006) or Zhang et al. (2000). Especially, a large class of the NC methods exploits linearization of nonlinear plants, e.g. Huba and Ondera (2009), an application of PID controllers, e.g. Tan et al. (2002), Bányász and Keviczky (2002) or factorization of nonlinear models of the plants on linear and nonlinear parts, e.g. Nakamura et al. (2002), Vallery et al. (2009) and Chyi-Tsong Chen1 et al. (2006).

In this paper, the CSTR control strategy is based on an application of the controller consisting of a static nonlinear part (SNP) and dynamic linear part (DLP). The static nonlinear part is obtained from simulated or measured steady-state characteristic of the CSTR, its inversion, polynomial approximation, and, subsequently, its differentiation. On behalf of development of the linear part, the SNP including the nonlinear model of the CSTR are approximated by a CT external linear model. For the CT ELM parameter estimation, an external delta model with the same structure as the CT model is used (see, e.g. Mukhopadhyay et al. (1992), Goodwin et al. (2001) and Stericker and Sinha (1993)). Then, the resulting CT controller is derived using the polynomial approach and pole assignment method, e.g. Kučera (1993). The simulations are performed on a nonlinear model of the CSTR with a consecutive exothermic reaction.

2. MODEL OF THE CSTR

Consider a CSTR with the first order consecutive exothermic reaction according to the scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ and with a perfectly mixed cooling jacket. Using the usual simplifications, the model of the CSTR is described by four nonlinear differential equations

$$\frac{dc_A}{dt} = -\left(\frac{q_r}{V_r} + k_1\right)c_A + \frac{q_r}{V_r}c_{Af} \tag{1}$$

$$\frac{dc_B}{dt} = -\left(\frac{q_r}{V_r} + k_2\right)c_B + k_1 c_A + \frac{q_r}{V_r}c_{Bf} \tag{2}$$

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

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

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 is the time, c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, q are volumetric flow rates, A_h is the heat exchange surface area and U is the heat transfer coefficient. The subscripts are denoted $(\cdot)_r$ for the reactant mixture, $(\cdot)_c$ for the coolant, $(\cdot)_f$ for feed (inlet) values and the superscript $(\cdot)^s$ for steady-state values. The reaction rates and the reaction heat are expressed as

$$k_j = k_{0j} \exp\left(\frac{-E_j}{RT_r}\right), \; j = 1, 2 \quad (5)$$

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B \quad (6)$$

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

Table 1. Parameters, inlet values and initial conditions.

$V_r = 1.2$ m^3 $V_c = 0.64$ m^3 $\rho_r = 985$ kg m^{-3} $\rho_c = 998$ kg m^{-3}	$c_{pr} = 4.05$ kJ kg^{-1}K^{-1} $c_{pc} = 4.18$ kJ kg^{-1}K^{-1} $A_h = 5.5$ m^2 $U = 43.5$ kJ m^{-2}min^{-1}K^{-1}
$k_{10} = 5.616 \cdot 10^{16}$ min^{-1} $k_{20} = 1.128 \cdot 10^{18}$ min^{-1} $h_1 = 4.8 \cdot 10^4$ kJ kmol^{-1}	$E_1/R = 13477$ K $E_2/R = 15290$ K $h_2 = 2.2 \cdot 10^4$ kJ kmol^{-1}
$c_{Af}^s = 2.85$ kmol m^{-3} $T_{rf}^s = 323$ K $q_r^s = 0.08$ m^{3}min^{-1}	$c_{Bf}^s = 0$ kmol m^{-3} $T_{cf}^s = 293$ K $q_c^s = 0.08$ m^{3}min^{-1}
$c_A^s = 1.5796$ kmol m^{-3} $T_r^s = 324.80$ K	$c_B^s = 1.1975$ kmol m^{-3} $T_c^s = 306.28$ K

In term of the practice, only the coolant flow rate can be taken into account as the control input. As the controlled output, the reactant temperature is considered. For the control purposes, the control input and the controlled output are defined as deviations from steady values

$$u(t) = q_c(t) - q_c^s, \quad y(t) = T_r(t) - T_r^s \quad (7)$$

The dependence of the reactant temperature on the coolant flow rate in the steady-state is in Fig.1.

In subsequent control simulations, the operating interval for q_c has been determined as

$$q_{c\min} \le q_c(t) \le q_{c\max} \quad (8)$$

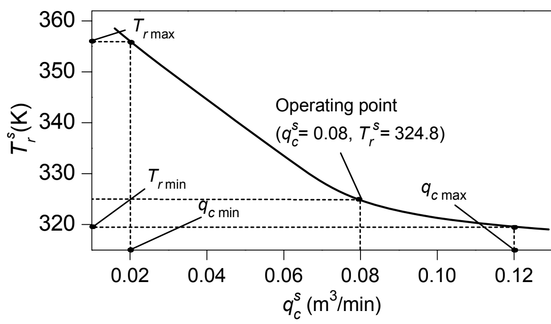

Fig. 1. Dependence of the reactant temperature on the coolant flow rate in the steady-state.

3. CONTROLLER DESIGN

As previously introduced, the controller consist of a static nonlinear part and a dynamic linear part as shown in Fig. 2.

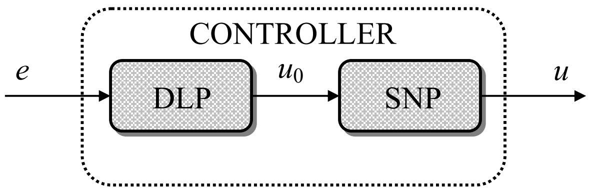

Fig. 2. The controller scheme.

The DLP creates a linear dynamic relation between the tracking error $e(t)$ and $u_0(t) = \Delta T_{rw}(t)$ which represents a difference of the reactant temperature adequate to its desired value. Evidently, for a well proposed SNP, the limit relation $\lim_{t\to\infty} u_0(t) = w$ holds.

Then, the SNP generates a static nonlinear relation betveen u_0 and a corresponding increment (decrement) of the coolant flow rate.

3.1 Nonlinear part of the controller

The SNP derivation appears from a simulated or measured steady-state charasteristics. From the purposes of a later polynomial approximation, the coordinates on the graph axis are defined as

$$\theta = \frac{q_c^s - q_{cL}}{q_{cL}}, \quad \xi = T_r^s - T_{rL}. \quad (9)$$

where q_{cL} is the lower bound in the interval

$$q_{cL} \le q_c^s \le q_{cU} \quad (10)$$

and, T_{rL} is the temperature corresponding to q_{cU}.

It can be recommended to select the interval (10) slightly longer than (8). In this paper, lower and upper values in (8) and (10) were chosen $q_{cL} = 0.016, q_{c\min} = 0.02, q_{c\max} = 0.12$ and $q_{cU} = 0.13$.

In term of the practice, it can be supposed that the measured data will be affected by measurement errors. The simulated steady-state characteristic that corresponds to reality is shown in Fig. 3.

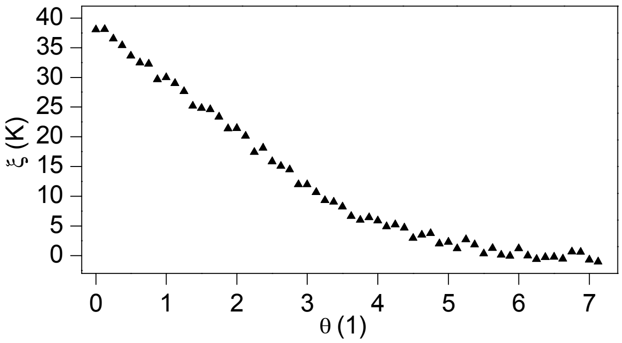

Fig. 3. Simulated characteristics $\xi = f(\theta)$.

Making the replacement of coordinates, the inverse of this characteristic can be approximated by a polynomial in the general form

$$\theta = a_0 + a_1 \xi + ... + a_{n-1} \xi^{n-1} + a_n \xi^n \, . \qquad (11)$$

The inverse characteristic accordant with Fig. 3 together with the fourth order approximate polynomial is in Fig. 4.

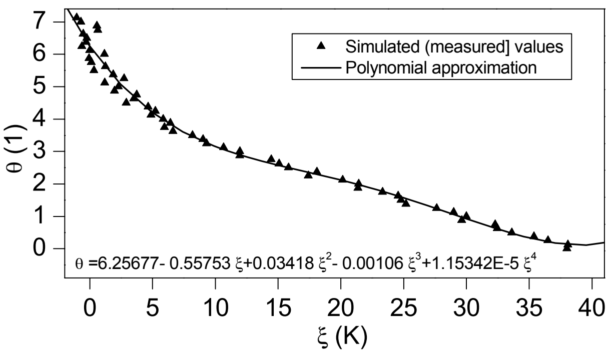

Fig. 4. Simulated and approximated inverse relation $\theta = \tilde{f}(\xi)$.

Now, a difference of the coolant flow rate $u(t) = \Delta q_c(t)$ in the output of the SNP can be computed for each T_r as

$$u(t) = \Delta q_c(t) = q_{cL} \left. \frac{d\theta}{d\xi} \right|_{\xi(T_r)} u_0(t) \qquad (12)$$

The derivative of the approximate polynomial is in Fig. 5.

3.2 CT external linear model of nonlinear elements

A structure of the CT ELM of the SNP in conjuction with the CSTR nonlinear model was chosen on the basis of step responses simulated in a neighbourhood of the operating point. The step responses for some step changes of u_0 are shown in Fig. 6. For all responses, the gain of the SNP+CSTR system has been computed as $g_s = \lim_{t \to \infty} \frac{y(t)}{u_0}$.

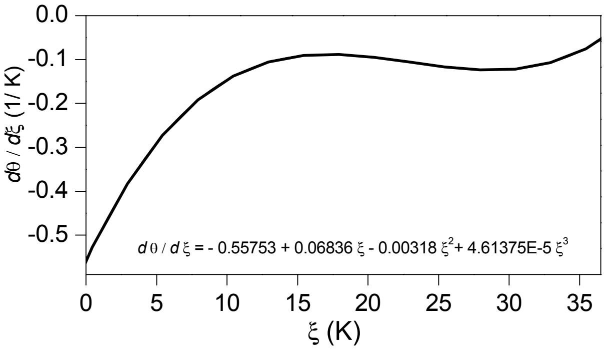

Fig. 5. Derivative of θ with respect to ξ.

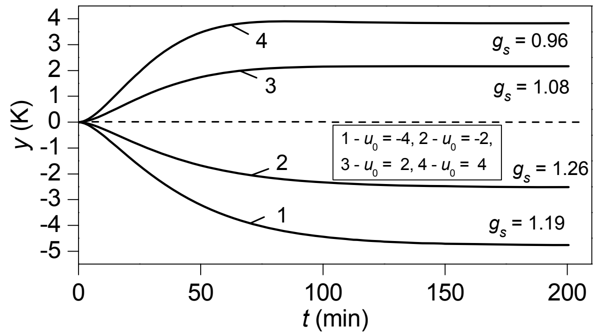

Fig. 6. Step responses of the SNP+CSTR.

Taking into account profiles of curves in Fig. 6 with zero derivatives for t = 0, the second order CT ELM has been chosen in the form of the second order linear differential equation

$$\ddot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_0 u_0(t) \qquad (13)$$

or, in the transfer function representation as

$$G(s) = \frac{Y(s)}{U_0(s)} = \frac{b_0}{s^2 + a_1 s + a_0} \, . \qquad (14)$$

3.3 Delta external linear model

Establishing the δ operator

$$\delta = \frac{q-1}{T_0} \qquad (15)$$

where q is the forward shift operator and T_0 is the sampling period, the delta ELM corresponding to (13) takes the form

$$\delta^2 y(t') + a_1' \delta y(t') + a_0' y(t') = b_0' u_0(t') \qquad (16)$$

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' of (16) reach the parameters a, b of the CT model (13) as proved in e.g. Stericker and Sinha (1993).

Substituting $t' = k - 2$, equation (16) may be rewriten to the form

$$\delta^2 y(k-2) + a_1' \delta y(k-2) + a_0' y(k-2) = b_0' u_0(k-2) \, . \qquad (17)$$

3.4 Delta model parameter estimation

Establishing the regression vector

$$\boldsymbol{\Phi}_\delta^T(k-1) = \left(\delta y(k-2)\ y(k-2)\ u_0(k-2)\right) \tag{18}$$

where

$$\delta y(k-2) = \frac{y(k-1) - y(k-2)}{T_0} \tag{19}$$

then, the vector of delta model parameters

$$\boldsymbol{\Theta}_\delta^T(k) = \left(a_1'\ a_0'\ b_0'\right) \tag{20}$$

is recursively estimated from the ARX model

$$\delta^2 y(k-2) = \boldsymbol{\Theta}_\delta^T(k)\,\boldsymbol{\Phi}_\delta(k-1) + \varepsilon(k) \tag{21}$$

where

$$\delta^2 y(k-2) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_0^2}. \tag{22}$$

The recursive estimation of delta model parameters was performed with the sampling interval T_0 = 0.2 min. Here, the recursive identification method with exponential and directional forgetting according to Rao and Unbehauen (2005) and Bobál et al. (2005) was used.

3.5 Linear part of the controller

The DLP is inserted into the control loop according to Fig. 7.

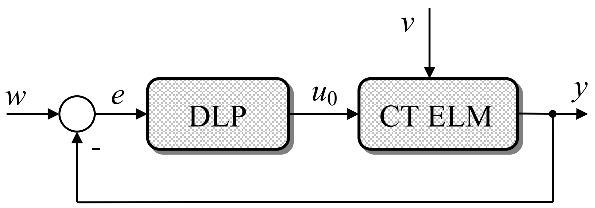

Fig. 7. Simplified scheme of the control loop.

In the scheme, w is the reference signal, v is the disturbance, y is the controlled output and u_0 is the input to the CT ELM. The transfer function G of the CT ELM is given by (14). Both the reference w and the disturbance v are considered to be step functions with transforms

$$W(s) = \frac{w_0}{s}, \quad V(s) = \frac{v_0}{s} \tag{23}$$

The transfer function of the DLP is in the form

$$Q(s) = \frac{U_0(s)}{E(s)} = \frac{q(s)}{p(s)} \tag{24}$$

where q and p are polynomials in s, and, $\deg q \le \deg p$.

The controller design described in this section stems from the polynomial approach. General conditions required to govern the control system properties are formulated as strong stability (in addition to the control system stability, also the stability of controllers is required), internal properness, asymptotic tracking of a step reference and step disturbance attenuation.

It is well known from the algebraic control theory that a controller which satisfies above requirements is in the polynomial ring given by a solution of the polynomial (Diophantine) equation

$$a(s)\,p(s) + b(s)\,q(s) = d(s) \tag{25}$$

with a stable polynomial $d(s)$ on the right side.

For step input signals w and v, the polynomial p is in the form

$$p(s) = s\,\tilde{p}(s). \tag{26}$$

The degrees of unknown polynomials in (25) and (26) are

$$\deg q = \deg a, \quad \deg \tilde{p} = \deg a - 1, \quad \deg d = 2\deg a.$$

Then, for the ELM (14), the controller transfer function takes the form

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

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

$$n(s) = s^2 + n_1 s + n_0 \tag{30}$$

with coefficients

$$n_0 = \sqrt{a_0^2}, \quad n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0}. \tag{31}$$

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

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ a_1 & b_0 & 0 & 0 \\ a_0 & 0 & b_0 & 0 \\ 0 & 0 & 0 & b_0 \end{pmatrix} \cdot \begin{pmatrix} p_0 \\ q_2 \\ q_1 \\ q_0 \end{pmatrix} = \begin{pmatrix} d_3 - a_1 \\ d_2 - a_0 \\ d_1 \\ d_0 \end{pmatrix} \tag{32}$$

where

$$\begin{aligned} d_3 &= n_1 + 2\alpha, \; d_2 = 2\alpha n_1 + n_0 + \alpha^2 \\ d_1 &= 2\alpha n_0 + \alpha^2 n_1, \; d_0 = \alpha^2 n_0 \end{aligned}. \tag{33}$$

Evidently, the controller parameters can be adjusted by the selectable parameter α. The complete adaptive control system is shown in Fig. 8.

4. CONTROL SIMULATIONS

The control simulations were performed in a neighbourhood of the operating point (q_c^s = 0.08 m^{3}min^{-1}, T_r^s = 324.8 K).

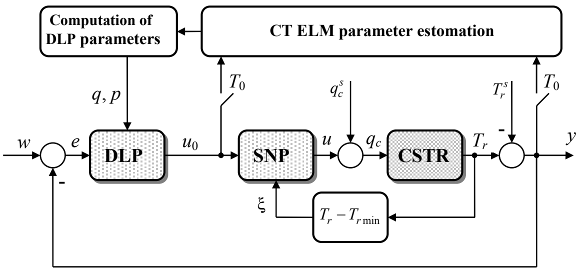

Fig. 8. Scheme of the nonlinear adaptive control.

For the start (the adaptation phase), a P controller with a small gain was used in all simulations.

The effect of the pole α on the control responses is transparent from Figs. 9, 10 and 11. Here, on the basis of precomputed simulations, two values of α were selected. The control results show sensitivity of the controlled output and the input signals to α. Obviously, careless selection of this parameter can lead to controlled output responses of a poor quality or even to unstability. Further, a increasing α leads to higher values and changes of the input signals.

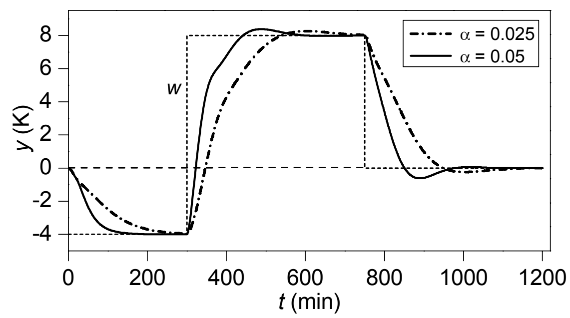

Fig. 9. Nonlinear adaptive control: Controlled output responses.

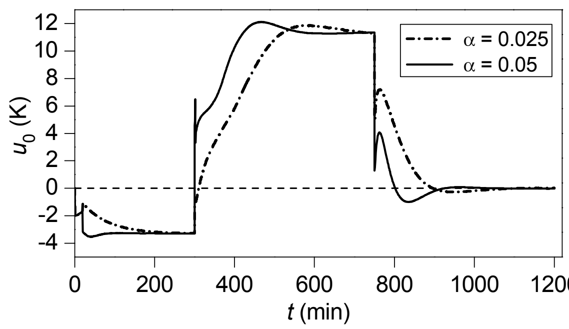

Fig. 10. Nonlinear adaptive control: Input signal to the SNP.

Evolution of the DLP parameters during control is shown in Fig. 12.

A presence of the integrating part in the DLP enables rejection of various step disturbances entering into the process. Here, step disturbances $\Delta c_{Af} = \pm 0.1\,\mathrm{kmol\,m^{-3}}$ at times $t_{v1} = 250\,\mathrm{min}$ and $t_{v2} = 550\,\mathrm{min}$ were injected into the CSTR. The DLP parameters were estimated only in the first (tracking) interval $t < 200$ min. The experiences of authors of this paper proved that an utilization of recursive identification using the delta model in the phase of a constant reference and in a presence of step disturbances decreases the control quality. From this reason, during interval $t \geq 200$ min, fixed DLP parameters were used. The controlled output responses are shown in Fig. 13.

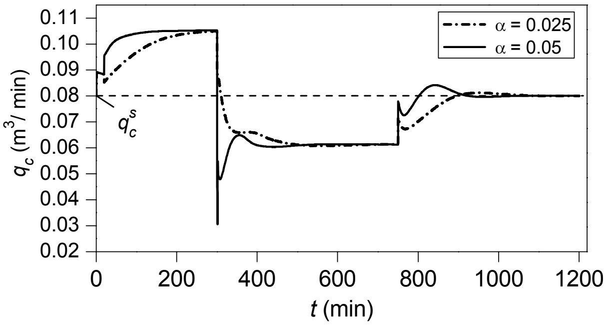

Fig. 11. Nonlinear adaptive control: Input to the CSTR.

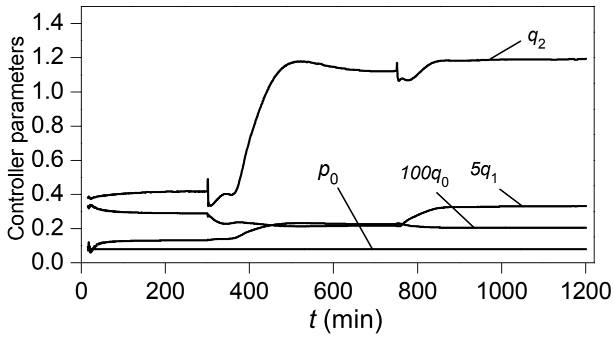

Fig. 12. Evolution of the DLP parameters during control.

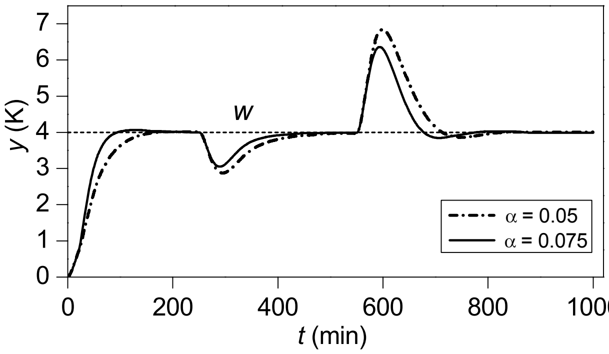

Fig. 13. Nonlinear adaptive control: Step disturbances rejection.

An influence of the SNP is evident from the control response shown in Fig. 14. Here, the standard adaptive control without the nonlinear part of the controller was used. The simulation has been performed under the same conditions as by above presented cases. A confrontation with responses in Fig. 9 shows that an application of the nonlinear control is suitable especially for greater changes of the reference signal.

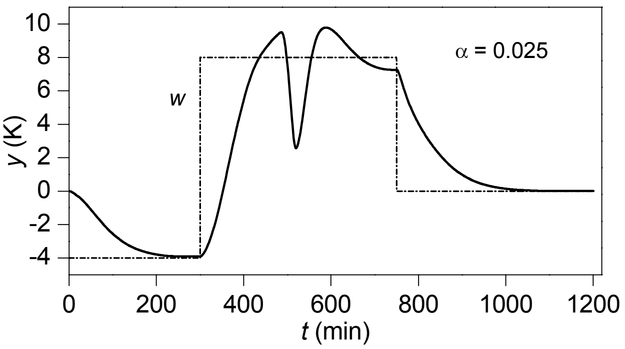

Fig. 14. Adaptive control without the SNP.

5. CONCLUSIONS

In this paper, one approach to the nonlinear continuous-time adaptive control of the reactant temperature in a continuous stirred tank reactor was proposed. The control strategy is based on a factorization of a controller into the linear and the nonlinear part. A design of the controller nonlinear part employs simulated or measured steady-state characteristics of the process and their additional modifications. Then, the system consisting of the controller nonlinear part and a nonlinear model of the CSTR is approximeted by a continuous time external linear model with parameters obtained through recursive parameter estimation of a corresponding delta model. The resulting continuous-time controller linear part is derived using the polynomial approach and given by a solution of a polynomial equation. Tuning of its parameters is possible via closed-loop pole assignment. The presented method has been tested by computer simulation on the nonlinear model of the CSTR with a consecutive exothermic reaction. Simulation results demonstrated an applicability of the presented control strategy and its usefulness especially for greater changes of input signals in strongly nonlinear regions. It can be expected that the described control strategy is also suitable for other similar technological processes such as tubular chemical reactors.

ACKNOWLEDGMENT

The authors wish to thank to the Ministry of Education of the Czech Republic (MSM7088352101) for financial support. This article was created with support of Operational Programme Research and Development for Innovations co-funded by the European Regional Development Fund (ERDF) and national budget of Czech Republic within the framework of the Centre of Polymer Systems project (reg.number: CZ.1.05/2.1.00/03.0111).

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