SIMULATION OF NONLINEAR ADAPTIVE CONTROL OF A TUBULAR CHEMICAL REACTOR

Petr Dostál [(a,b)], Jiří Vojtěšek [(b)], Vladimír Bobál [(a,b)]

[(a)] Centre of Polymer Systems, [(b)] Department of Process Control
Tomas Bata University in Zlin
nam. T. G. Masaryka 5555, 760 01 Zlin
Czech Republic.

{dostalp;vojtesek;bobal}@fai.utb.cz

ABSTRACT
The paper presents design and simulation results of nonlinear adaptive control of a tubular chemical reactor. The control strategy is based on factorization of the controller on an adaptive dynamic linear part and a static nonlinear part. The static nonlinear part is derived using simulated steady-state characteristics of the process and its subsequent inversion and approximation. The linear part consisting of two linear feedback controllers results from an approximation of nonlinear elements in the control system by an external linear model with recursively estimated parameters. The control law is derived via the polynomial approach and the pole placement method.

Keywords: tubular chemical reactor, nonlinear model, external linear model, parameter estimation, pole assignment

1. INTRODUCTION

From the system theory point of view, tubular chemical reactors (TCRs) belong to a class of nonlinear distributed parameter systems. Their mathematical models are described by sets of nonlinear partial differential equations (PDRs). The methods of modelling and simulation of such processes are described eg. in (Luyben 1989; Ingham et al. 1994).

It is well known that the control of chemical reactors, and, TCRs especially, often represents very complex problem. The control problems are due to the process nonlinearity, its distributed nature, 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, the time delay 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.

An effective approach to the control of nonlinear processes utilizes methods of the nonlinear control (NC) in conjunction with linear adaptive control Several modifications of the NC theory are described in e.g. (Astolfi et al. 2008; Vincent and Graham 1997). Especially, a large class of the NC methods exploits linearization of nonlinear plants, e.g. (Huba and Ondera 2009), 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. (Chyi-Tsong Chen1 et al. 2006; Vörös 2008; Sung and Lee 2004).

In this paper, the TCR control strategy is based on application of the controller consisting of a static nonlinear part (SNP) and dynamic linear part (DLP). With respect to practical possibilities of a measurement and control, the mean reactant temperature is chosen as the controlled output, and, the coolant flow rate as the control input. The static nonlinear part is obtained from simulated steady-state characteristic of the TCR, its inversion, approximation and, subsequently, its differentiation. On behalf of development of the linear part, the SNP including the nonlinear model of the TCR is approximated by a continuous-time external linear model (CT ELM), e.g. (Dostál et al. 2009) with parameters estimated via corresponding delta model, see, e.g. (Middleton and Goodwin 1990; Mukhopadhyay et al. 1992; Stericker and Sinha 1993). The control system with two feedback controllers is used according to (Dostál et al. 2007). Resulting CT controllers are derived using the polynomial approach and the pole assignment method, e.g. (Kučera 1993). The simulations are performed on a nonlinear model of the TCR with a consecutive exothermic reaction.

2. MODEL OF THE REACTOR

An ideal plug-flow tubular chemical reactor with a simple exothermic consecutive reaction 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 is significant. All densities, heat capacities, and heat transfer coefficients are assumed to be constant. Under above assumptions, the reactor model can be described by five PDRs in the form

$$\frac{\partial c_A}{\partial t} + v_r \frac{\partial c_A}{\partial z} = -k_1 c_A \tag{1}$$

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

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

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

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

with initial conditions

$c_A(z,0) = c_A^s(z)$, $c_B(z,0) = c_B^s(z)$, $T_r(z,0) = T_r^s(z)$, $T_w(z,0) = T_w^s(z)$, $T_c(z,0) = T_c^s(z)$

and boundary conditions

$c_A(0,t) = c_{A0}(t)$ (kmol/m^3), $c_B(0,t) = c_{B0}(t)$ (kmol/m^3), $T_r(0,t) = T_{r0}(t)$ (K), $T_c(L,t) = T_{cL}(t)$ (K).

Here, t is the time, z is the axial space variable, c are concentrations, T are temperatures, v are fluid velocities, d are diameters, ρ are densities, c_p are specific heat capacities, U are 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

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

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

where k_0 are pre-exponential factors, E are activation energies, (- ΔH_r) are in the negative considered reaction entalpies, and R is the gas constant.

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

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

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

From the system engineering point of view, $c_A(L,t) = c_{A\mathrm{out}}$, $c_B(L,t) = c_{B\mathrm{out}}$, $T_r(L,t) = T_{r\mathrm{out}}$ and $T_c(0,t) = T_{c\mathrm{out}}$ 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, the coolant flow rate can be taken into account as the control variable, whereas other inputs can be accepted as disturbances. The mean reactant temperature given by

$$T_m(t) = \frac{1}{L}\int_0^L T_r(z,t)\, dz \tag{9}$$

is considered as the controlled output.

The values of parameters and steady-state inputs used in simulations are in Table 1.

Table 1: Parameters and Steady-State Inputs

L = 8 m	n_1 = 1200
d_1 = 0.02 m	d_2 = 0.024 m
d_3 = 1 m	
ρ_r = 985 kg/m^3	c_{pr} = 4.05 kJ/kg K
ρ_w = 7800 kg/m^3	c_{pw} = 0.71 kJ/kg K
ρ_c = 998 kg/m^3	c_{pc} = 4.18 kJ/kg K
U_1 = 2.8 kJ/m^{2}s K	U_2 = 2.56 kJ/m^{2}s K
k_{10} = 5.61·10^{16} 1/s	k_{20} = 1.128·10^{18} 1/s
E_1/R = 13477 K	E_2/R = 15290 K
(-ΔH_{r1}) = 5.8·10^4 kJ/kmol	(-ΔH_{r2}) = 1.8·10^4 kJ/kmol
$c_{A0}^s = 2.85$ kmol/m^3	$c_{B0}^s = 0$ kmol/m^3
$T_{r0}^s = 323$ K	$T_{c0}^s = 293$ K
$q_r^s = 0.15$ m^3/s	

3. COMPUTATION MODELS AND STEADY-STATE CHARACTERISTICS

For computation of both steady-state and dynamic characteristics, the finite diferences method is employed. The procedure is based on substitution of the space interval $z \in <0, L>$ by a set of discrete node points $\{z_i\}$ for i = 1, … , 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 dependence of the mean reactant temperature on the coolant flow rate in the steady-state is in Figure 1. In subsequent control simulations, the operating interval for q_c has been determined as

$$q_{c\min} \le q_c(t) \le q_{c\max} \tag{10}$$

With regard to the purposes of a latter steady-state characteristic approximation, the values q_{cL} and q_{cU} are established that denote the lower and upper bound of q_c^s used for the approximation. Their values together with values in (10), and, to them corresponding temperatures are in Table 2.

Table 2: Variables Used in Control and Approximation

$q_{cL} = 0.18$	$q_{c\min} = 0.2$
$T_{mU} = 346.66$	$T_{m\max} = 344.57$
$q_{c\max} = 0.4$	$q_{cU} = 0.42$
$T_{m\min} = 320.30$	$T_{mL} = 319.80$

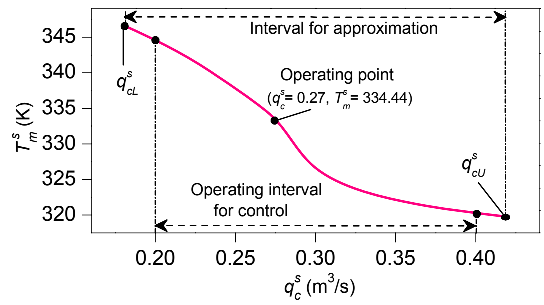

Figure 1: Dependence of the Reactant Temperature on the Coolant Flow Rate in the Steady-State

4. CONTROLLER DESIGN

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

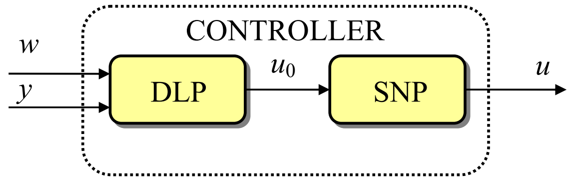

Figure 2: The Controller Scheme

Here, the control input and the controlled output variables are considered in the form

$$u(t) = q_c(t) - q_c^s\,, \quad y(t) = T_m(t) - T_m^s \tag{11}$$

The DLP creates a linear dynamic relation $u_0(t) = \Delta T_{mw}(t)$ which represents a difference of the mean reactant temperature adequate to its desired value. Then, the SNP generates a static nonlinear relation betveen u_0 and a corresponding increment (decrement) of the coolant flow rate.

4.1. Nonlinear Part of the Controller

The SNP derivation appears from a simulated or measured steady-state charasteristic. There, the coordinates on the graph axis are defined as

$$\gamma = 10\frac{q_c^s - q_{cL}}{q_{cL}}\,, \quad \xi = T_m^s - T_{mL} \tag{12}$$

where

$$q_{cL} \le q_c^s \le q_{cU} \tag{13}$$

Expressions (12) lead to coordinates with the magnitudes in the same order. This property is useful for latter approximation. 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 Figure 3.

Making the change of coordinates, the inverse of this characteristic can be approximated by a function from the ring of polynomial, exponential, rational, eventually, by other type functions. Here, the

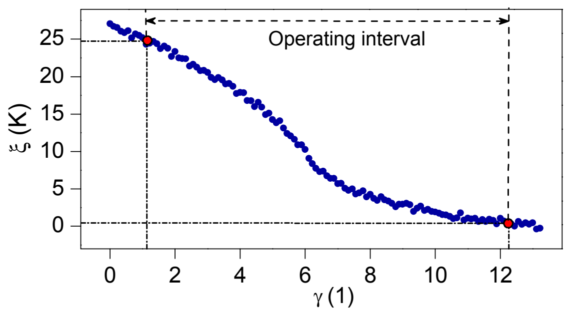

Figure 3: Simulated Characteristics ξ = *f*(γ)

polynomial approximate function has been found using the least square method in the form

$$\gamma = 12.9516 - 1.9062\,\xi + 0.2151\,\xi^2 - 0.01244\,\xi^3 + \\ + 3.288\cdot 10^{-4}\,\xi^4 - 3.3535\cdot 10^{-6}\,\xi^5 \tag{14}$$

The inverse characteristic together with its polynomial approximation is in Figure 4.

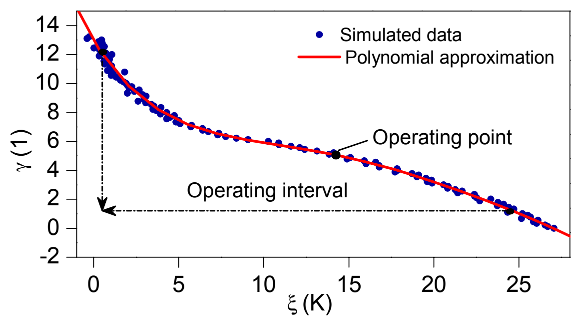

Figure 4: Simulated Inverse Characteristics with Polynomial Approximation

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_m as

$$u(t) = \Delta q_c(t) = q_{cL}\left(\frac{d\gamma}{d\xi}\right)_{\xi(T_m)} u_0(t)\,. \tag{15}$$

The derivative of γ with respect to ξ takes the form

$$\frac{d\gamma}{d\xi} = -1.9062 + 0.4302\,\xi - 0.03732\,\xi^2 + \\ + 1.3152\cdot 10^{-3}\,\xi^3 - 1.6768\cdot 10^{-5}\,\xi^4\,. \tag{16}$$

Its plot is shown in Figure 5.

4.2. CT and Delta External Linear Model of Nonlinear Elements

A choice of the CT ELM structure does not stem from known structure of the model (1) – (5) but from a character of simulated step responses shown in Figure 6.

It is well known that in adaptive control a controlled process of a higher order can be approximated by a linear model of a lower order with variable parameters.

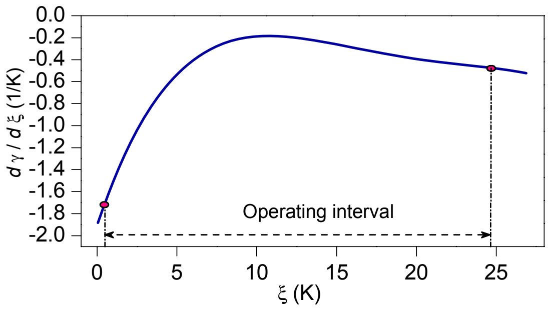

Figure 5: Derivative of γ with Respect to ξ

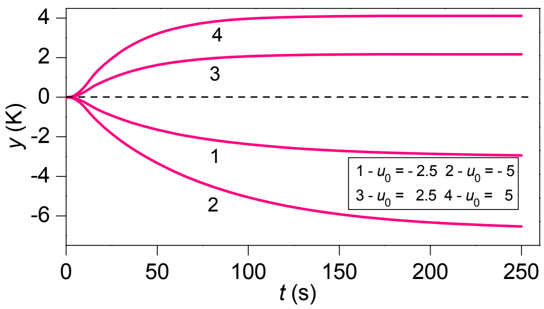

Figure 6: NPC + TCR Step Responses

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

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

and, in the complex domain, as the transfer function

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

Establishing the δ operator

$$\delta = \frac{q-1}{T_0} \tag{19}$$

where q is the forward shift operator and T_0 is the sampling period, the delta ELM corresponding to (17) takes the form

$$\delta^2 y(t') + a_1' \delta y(t') + a_0' y(t') = b_0' u(t') \tag{20}$$

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 (17), (18).

4.3. Delta Model Parameter Estimation

Substituting $t' = k - 2$, equation (20) can be rewriten to the form

$$\delta^2 y(k-2) + a_1' \delta y(k-2) + a_0' y(k-2) = b_0' u(k-2)\,. \tag{21}$$

Establishing the regression vector

$$\boldsymbol{\Phi}_\delta^T(k-1) = \left(-\delta y(k-2) \quad -y(k-2) \quad u(k-2)\right) \tag{22}$$

where

$$\delta y(k-2) = \frac{y(k-1) - y(k-2)}{T_0} \tag{23}$$

the vector of delta model parameters

$$\boldsymbol{\Theta}_\delta^T(k) = \left(a_1' \; a_0' \; b_0'\right) \tag{24}$$

is recursively estimated by the least squares method with exponential and directional forgetting (Bobál et al. 2005) from the ARX model

$$\delta^2 y(k-2) = \boldsymbol{\Theta}_\delta^T(k)\boldsymbol{\Phi}_\delta(k-1) + \varepsilon(k) \tag{25}$$

where

$$\delta^2 y(k-2) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_0^2}\,. \tag{26}$$

4.4. Linear Part of the Controller

The control system with two feedback controllers is depicted in Fig. 7. In the scheme, w is the reference signal, v denotes the load disturbance, e the tracking error, u_0 output of controllers, u the control input and y the controlled output. The transfer function $G(s)$ of the CT ELM is given by (18). The reference w and the disturbance v are considered as step functions.

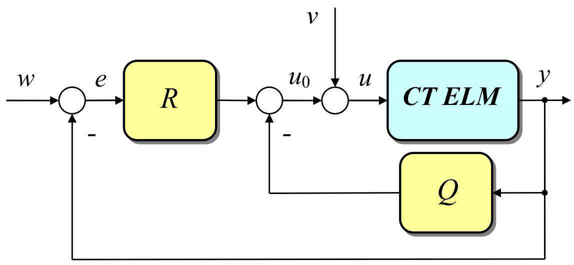

Figure 7: Control System with Two Feedback Controllers

Both feedback controllers can be derived using the polynomial approach. The general requirements on the control system are formulated as its internal properness and stability, asymptotic tracking of the reference and load disturbance attenuation. The procedure to derive admissible controllers is presented in detail in e.g. (Dostál et al. 2005).

Main results can briefly be performed as follows: The transfer functions of resulting controllers that fulfil above requirements take forms

$$Q(s) = \frac{q(s)}{p(s)} = \frac{q_2 s + q_1}{s + p_0}$$
$$R(s) = \frac{r(s)}{s\,p(s)} = \frac{r_2 s^2 + r_1 s + r_0}{s(s + p_0)}\,. \tag{27}$$

where polynomials q, r and p are obtained by a solution of polynomial equations

$$a(s) s\, p(s) + b(s)\, t(s) = d(s) \tag{28}$$

$$t(s) = r(s) + s\, q(s) \tag{29}$$

where $p(s) = s + p_0$ and $t(s) = t_2 s^2 + t_1 s + t_0$.
Relations among coefficients of polynomials *t*, *r* and *q* are given as

$$r_0 = t_0,\ r_1 = \beta_1 t_1,\ r_2 = \beta_2 t_2,$$
$$q_1 = (1-\beta_1) t_1,\ q_2 = (1-\beta_2) t_2 \tag{30}$$

where $\beta_i \in \langle 0,1 \rangle$ are selectable coefficients distributing a weight between numerators of transfer functions *Q* and *R*.
The controller parameters depend upon coefficients of the polynomial *d*. In this paper, the polynomial *d* with roots determining the closed-loop poles is chosen as

$$d(s) = n(s)(s+\alpha)^2 \tag{31}$$

where $n(s) = s^2 + n_1 s + n_0$ is a stable polynomial obtained by spectral factorization

$$a^*(s) a(s) = n^*(s) n(s) \tag{32}$$

and α is the selectable parameter.
Note that a choice of *d* in the form (31) provides the control of a good quality for aperiodic controlled processes.
The coefficients *n* then are expressed as

$$n_0 = \sqrt{a_0^2},\quad n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0} \tag{33}$$

and, the parameters p_0 and *t* are given by a solution of the polynomial equation (28).
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 (30).
The complete control system is shown in Figure 8.

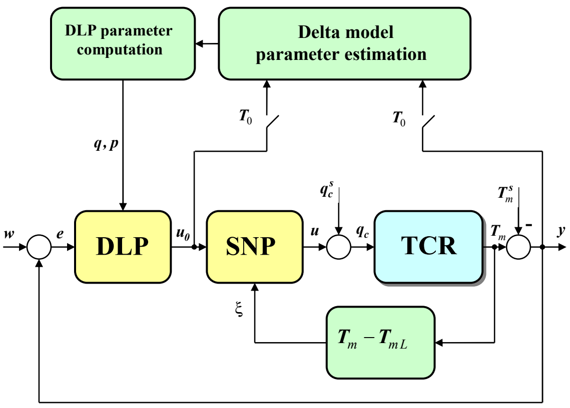

Figure 8: Complete Control System.

5. SIMULATION RESULTS

The control simulations were performed in a neighbourhood of the operating point (q_c^s = 0.27 m^{3}min^{-1}, T_r^s = 324.8 K). For the start (the adaptation phase), the DLP as 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 Figures 9 and 10. Here, on the basis of precomputed simulations, three values of *α* were selected. The control results show sensitivity of the output and the input signals to α. Obviously, careless selection of this parameter can lead to controlled outputs with overshoots and oscillations. Moreover, an increasing *α* leads to higher values and changes of the input signal. This fact can be important in control of some reactors where expressive input changes are undesirable.

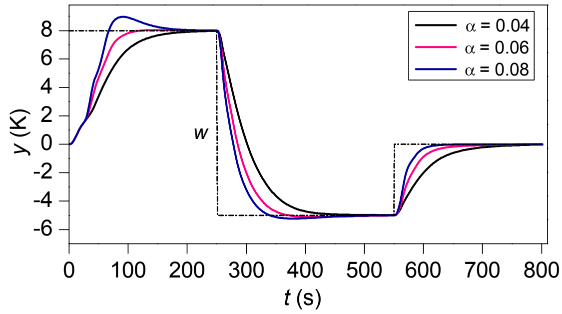

Figure 9: Controlled Output Responses for Various α

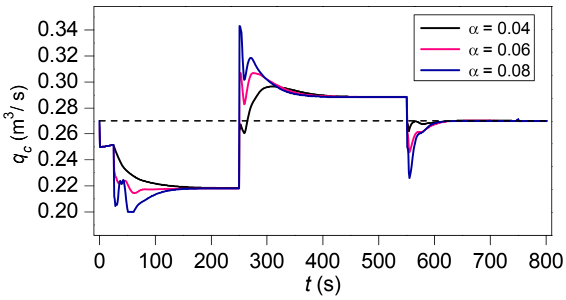

Figure 10: Coolant Flow Rate Responses for Various α

The controlled output responses documenting an effect of the parameter β_1 are in Figure 11. There, a higher value of β_1 speeds the control.

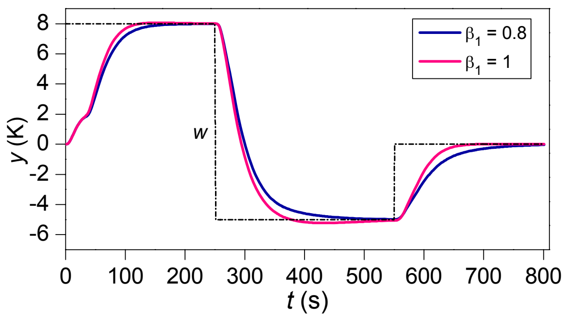

Figure 11: Controlled Output Responses: Effect of β_1 ($\beta_2 = 0$)

A comparison of the nonlinear adaptive control with the standard adaptive control without the nonlinear part can be seen in Fig. 12. The simulations were performed for α = 0.05. The responses document priority of the nonlinear control especially for greater changes of the reference signal.

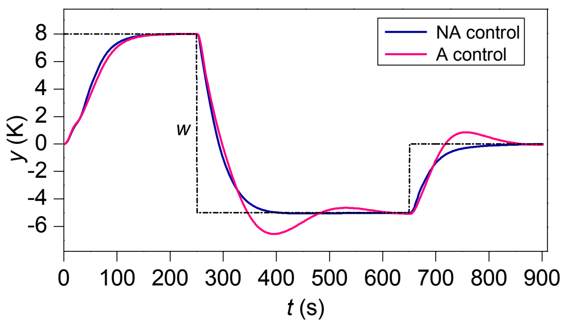

Figure 12: Comparison of Nonlinear Adaptive Control (NA) with Standard Adaptive Control (A).

6. CONCLUSIONS

In this paper, one approach to the nonlinear continuous-time adaptive control of the mean reactant temperature in a tubular chemical reactor was proposed. The control strategy is based on a factorization of a controller into the linear and the nonlinear parts. 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 TCR is approximeted by a continuous time external linear model with parameters recursively estimated via corresponding delta model. The resulting linear part consist of two feedback CT controllers. Tuning of their parameters is possible by selectable parameters α and β. The presented method has been tested by computer simulations on the nonlinear model of the TCR.

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