

USE OF NONLINEAR THEORY IN ADAPTIVE CONTROL OF CHEMICAL REACTOR

Jiri Vojtesek^(a), Petr Dostal^(a)

^(a)Department of Process Control, Faculty of Applied Informatics,
Tomas Bata University in Zlin, Nad Stranemi 4511, 76005 Zlin, Czech Republic

^(a)vojtesek@fai.utb.cz, dostalp@fai.utb.cz

ABSTRACT

This contribution is focused on the improvement of the adaptive control of the nonlinear process. The method used here is based on the separation of the controller to the linear and nonlinear part where the nonlinear part comes from the steady-state analysis and the linear part uses the External Linear Model (ELM) as a linear representation of the nonlinear parts in the loop. Parameters of the ELM are estimated recursively with the use of delta models as a special types of discrete-time models. The controller synthesis uses a polynomial approach with the pole-assignment method which satisfies basic control requirements such as stability, a reference signal tracking and disturbance attenuation. The proposed methods are tested by the simulations on a mathematical model of the Continuous Stirred Tank Reactor (CSTR) as a typical member of nonlinear systems with lumped parameters.

Keywords: nonlinear adaptive control, recursive identification, CSTR, polynomial approach, pole-assignment method

1. INTRODUCTION

The adaptive control (Åström and Wittenmark 1989) is relatively old but still commonly used control method with strong background. The basic idea of adaptive control comes from the nature and human living where all living organisms “adapts” behavior to the actual state and the living environment. Transferred to the control theory, the adaptive controller adapts parameters or the structure to parameters of the controlled plant according to the selected criterion (Bobal et al. 2005).

The adaptive approach here is based on choosing an external linear model (ELM) of the original nonlinear system whose parameters are recursively identified during the control. This strategy was also presented for example in (Vojtesek and Dostal 2010) and (Vojtesek et al. 2011).

There are some disadvantages which could occur during the simulation experiments. The first problem was with the recursive identification at the beginning of the control when the controller does not have any a priori information about the system. Insensitive choice of starting values for the identification could lead to the suboptimal or unstable results. One solution how to

overcome this feature is to limit the action value, e.g. input to the system between some boundaries. The question is: What are the right boundaries? Or, what if these boundaries are too strict/liberal?

The control method used here is based on the combination of the adaptive control and nonlinear control. Theory of nonlinear control (NC) can be found for example in (Astolfi et al. 2008) and (Vincent and Grantham 1997), the factorization of nonlinear models of the plants on linear and nonlinear parts is described in (Nakamura et al. 2002) and (Sung and Lee 2004). The controller consists of a static nonlinear part (SNP) and a dynamic linear part (DLP). The static part is obtained from the steady-state characteristic of the system, its inversion, suitable approximation and its derivative. The linear part is then described by the external linear model with the use of delta (δ -) models (Middleton and Goodwin 2004) as a special type of discrete-time models parameters of which approaches to the continuous ones for the small sampling period (Stericker and Sinha 1993).

The polynomial approach (Kucera 1993) included in the control synthesis can be used for systems with negative properties from the control point of view such as nonlinear systems, non-minimum phase systems or systems with time delays. Moreover, the pole-placed method with spectral factorization satisfies basic control requirements such as disturbance attenuation, stability and reference signal tracking. The resulting controller is hybrid because polynomial synthesis is made for continuous-time but recursive identification runs on the delta-model, which belongs to the class of discrete-time models.

Chemical reactors are equipment widely used not only in the chemical industry for production of various products. The mathematical model of the Continuous Stirred-Tank Reactor used in this work is typical nonlinear system described mathematically by the set of two nonlinear ordinary differential equations (ODE) (Gao et al. 2002). As it is described in (Vojtesek and Dostal 2010), this system has two stable and one unstable steady-state which could lead to very unstable or suboptimal output responses with the use of conventional control methods.

All simulations were done on the mathematical simulation software Matlab, version 7.0.3.

2. CONTROLLED PLANT

The controlled process under the consideration is the continuous stirred tank reactor (CSTR) with the spiral cooling in the jacket. The scheme of the system can be found in Figure 1.

The complete mathematical description of the process is very complex and we must introduce some simplifications. At first, we expect that reactant is perfectly mixed and reacts to the final product with the concentration $c_A(t)$. The heat produced by the reaction is represented by the temperature of the reactant $T(t)$. Furthermore we also expect that volume, heat capacities and densities are constant during the control.

A mathematical model of this system is derived from the material and heat balances of the reactant and cooling. The resulted model is then a set of two Ordinary Differential Equations (ODEs) (Gao et al. 2002):

$$\frac{dT}{dt} = a_1 \cdot (T_0 - T) + a_2 \cdot k_1 \cdot c_A + a_3 \cdot q_c \cdot \left(1 - e^{\frac{a_4}{T}} \right) \cdot (T_0 - T) \quad (1)$$

$$\frac{dc_A}{dt} = a_1 \cdot (c_{A0} - c_A) - k_1 \cdot c_A$$

where a_{1-4} are constants computed as

$$a_1 = \frac{q}{V}; a_2 = \frac{-\Delta H}{\rho \cdot c_p}; a_3 = \frac{\rho_c \cdot c_{pc}}{\rho \cdot c_p \cdot V}; a_4 = \frac{-h_a}{\rho_c \cdot c_{pc}} \quad (2)$$

In previous equations, variable denotes time, T is used for temperature of the reactant, V is volume of the reactor, c_A represents concentration of the product, q and q_c are volumetric flow rates of the reactant and cooling respectively. Indexes $(\cdot)_0$ denote inlet values of the variables and $(\cdot)_c$ is used for variables related to the cooling.

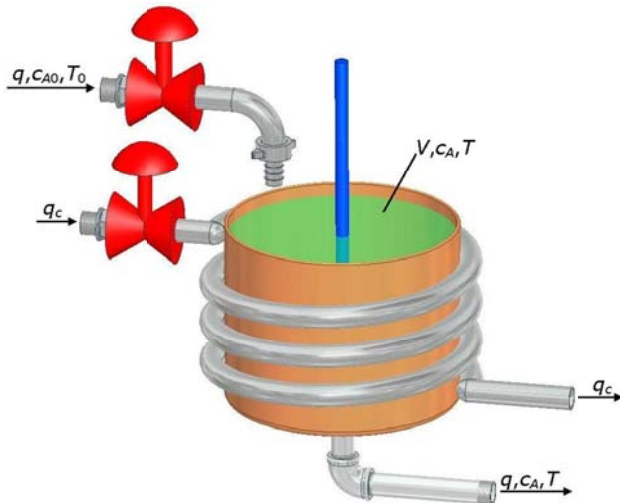


Figure 1: Continuous Stirred Tank Reactor

The fixed values of the system are shown in Table 1 (Gao et al. 2002).

Table 1: Fixed parameters of the reactor

Reactant's flow rate	$q = 100 \text{ l.min}^{-1}$
Reactor's volume	$V = 100 \text{ l}$
Reaction rate constant	$k_0 = 7.2 \cdot 10^{10} \text{ min}^{-1}$
Activation energy to R	$E/R = 1 \cdot 10^4 \text{ K}$
Reactant's feed temperature	$T_0 = 350 \text{ K}$
Reaction heat	$\Delta H = -2 \cdot 10^5 \text{ cal.mol}^{-1}$
Specific heat of the reactant	$c_p = 1 \text{ cal.g}^{-1} \cdot \text{K}^{-1}$
Specific heat of the cooling	$c_{pc} = 1 \text{ cal.g}^{-1} \cdot \text{K}^{-1}$
Density of the reactant	$\rho = 1 \cdot 10^3 \text{ g.l}^{-1}$
Density of the cooling	$\rho_c = 1 \cdot 10^3 \text{ g.l}^{-1}$
Feed concentration	$c_{A0} = 1 \text{ mol.l}^{-1}$
Heat transfer coefficient	$h_a = 7 \cdot 10^5 \text{ cal.min}^{-1} \cdot \text{K}^{-1}$

The nonlinearity of the model can be found in relation for the reaction rate, k_1 , which is computed from Arrhenius law:

$$k_1 = k_0 \cdot e^{\frac{-E}{R \cdot T}} \quad (3)$$

where k_0 is the reaction rate constant, E denotes an activation energy and R is a gas constant.

The static analysis of this system is described in detail for example in (Vojtesek and Dostal 2010). The most important result of the steady-state analysis can be found in the complexity of the system, it has three steady-states – one unstable (N_1) and two stable (S_1 and S_2). This special feature is shown in Figure 2 which represents values of the reactant (Q_r) and cooling (Q_c) heats for the working point represented by the volumetric flow rates $q = 100 \text{ l.min}^{-1}$ and $q_c = 80 \text{ l.min}^{-1}$ and various values of the temperature $T = \langle 300, 500 \rangle \text{ K}$.

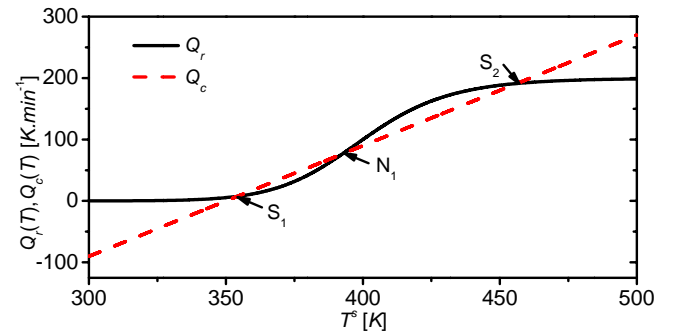


Figure 2: Heat balance inside the reactor

The steady-state values of the state variables in all three steady-states are:

$$\begin{aligned} S_1 : & \quad T^S = 354.23 \text{ K} & c_A^S = 0.9620 \text{ mol.l}^{-1} \\ N_1 : & \quad T^S = 392.45 \text{ K} & c_A^S = 0.6180 \text{ mol.l}^{-1} \\ S_2 : & \quad T^S = 456.25 \text{ K} & c_A^S = 0.0439 \text{ mol.l}^{-1} \end{aligned} \quad (4)$$

It is clear, that the second operating point S_2 has better efficiency (95.6 % reacts) for the same input

settings than on the point S_1 (3.8 % reacts). This is the main reason why we have chosen this second steady-state in this work. The static analysis for the different volumetric flow rate of the coolant

$$q_{c,min} \leq q_c \leq q_{c,max} \quad (5)$$

was done. The $q_{c,min}$ and $q_{c,max}$ denotes minimal and maximal values of the volumetric flow rate of the coolant and their values are $q_{c,min} = 20 \text{ l.min}^{-1}$ and $q_{c,max} = 100 \text{ l.min}^{-1}$. The results are shown in Figure 3.

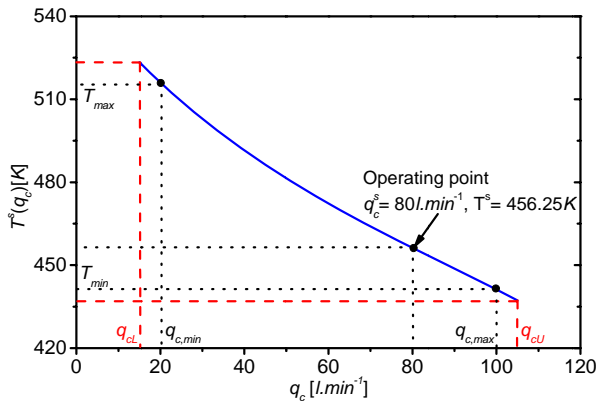


Figure 3: Static analysis of the reactor

3. NONLINEAR CONTROLLER

The controller here is divided into a static nonlinear part (SNP) and a dynamic linear part (DLP) – see Figure 4.

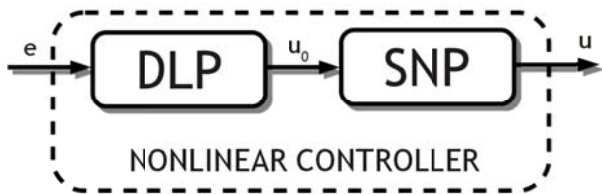


Figure 4: The scheme of the nonlinear controller

The dynamic part DLP defines linear dynamic relation between input to the nonlinear part $u_0(t)$ and the difference between actual and desired reactant temperature $T_w(t)$, i.e.

$$u_0(t) = \Delta T_w(t) \quad (6)$$

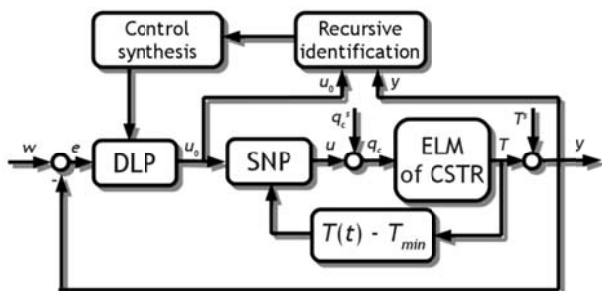


Figure 5: The control scheme

The static part SNP describes nonlinear relation between $u_0(t)$ and corresponding change of the input volumetric flow rate of the coolant $\Delta q_c(t)$.

The interconnection of the controller and the controller plant can be found in the following Figure 5.

3.1. Static Nonlinear Part (SNP)

The SNP at it is comes from the static analysis displayed in Figure for volumetric flow rate between lower bound $q_{cl} = 15 \text{ l.min}^{-1}$ and upper bound $q_{cU} = 105 \text{ l.min}^{-1}$ and we introduce new x - and y -axis coordinates ω and ψ defined as

$$\omega = \frac{q_c^s - q_{cl}}{q_{cl}} [-]; \psi = T^s - T_{min}^s [K] \quad (7)$$

where T_{min}^s represents the lowest value of the steady-state reactant temperature, i.e. T^s for the volumetric flow rate in the upper bound, q_{cU} , in this case.

The measured data on the real model are usually affected by the measurement errors. These errors are here simulated by the random white-noise errors. The steady-state characteristic recomputed to the new coordinates γ and ψ is then shown in Figure 6.

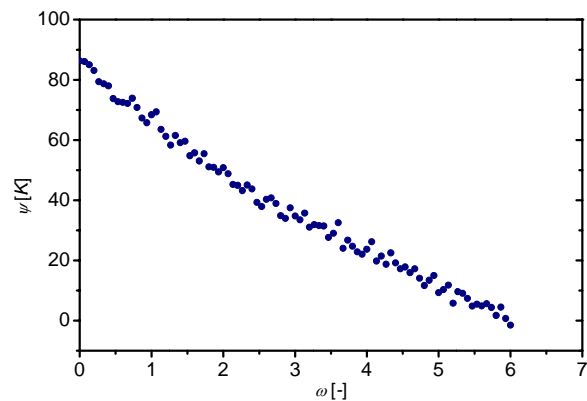


Figure 6: Simulated characteristic $\psi = f(\omega)$

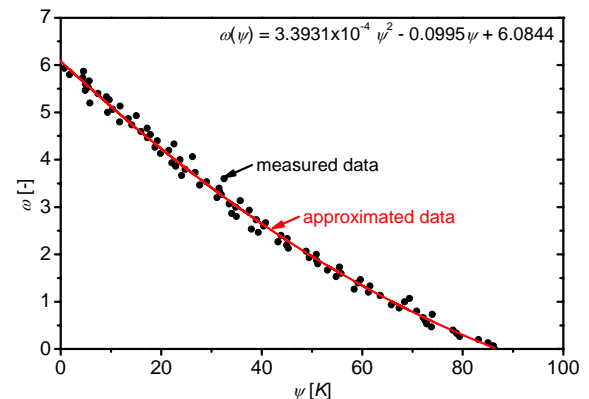


Figure 7: Simulated (dotted) and approximated (line) characteristic $\omega = f(\psi)$

The inverse of this steady-state characteristic is shown in Figure 7 and the resulted simulated data could

be approximated by several functions from the ring of polynomial, exponential, rational etc. functions. In our case, the second order polynomial was used for the approximation of the noised data. The resulted polynomial has form

$$\omega(\psi) = 3.3931 \times 10^{-4} \psi^2 - 0.0995\psi + 6.0844 \quad (8)$$

and as it can be seen in Figure 7, this function approximates the data in suitable way.

The difference of the input volumetric flow rate of the coolant $u(t) = \Delta q_c(t)$ in the output from the nonlinear part can be computed

$$u(t) = \Delta q_c(t) = q_{cl} \left(\frac{d\omega}{d\psi} \right)_{\psi(T)} u_0(t) \quad (9)$$

The derivative $d\omega/d\psi$ in the previous equation is computed for each temperature of the reactant T from the derivative of the function odkaz, i.e.

$$\frac{d\omega}{d\psi} = 6.7861 \times 10^{-4} \psi - 0.0995 \quad (10)$$

3.1.1. External Linear Model (ELM) of CSTR

The dynamic behavior of the system shows that this system could be represented by the second order transfer function with the relative order one:

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b(s)}{a(s)} = \frac{b_1s + b_0}{s^2 + a_1s + a_0} \quad (11)$$

This ELM belongs to the class of continuous-time (CT) models. The identification of such processes is not very easy. One way, how we can overcome this problem is the use of so called δ -model. This model belongs to the class of discrete models but its parameters are close to the continuous ones for very small sampling period as it proofed in (Stericker and Sinha 1993).

The δ -model introduces a new complex variable γ computed as (see (Mukhopadhyay et al. 1992)):

$$\gamma = \frac{z-1}{\beta \cdot T_v \cdot z + (1-\beta) \cdot T_v} \quad (12)$$

where β is an optional parameter from the interval $0 \leq \beta \leq 1$ and T_v denotes a sampling period. It is clear that we can obtain infinite number of δ -models for various β . A so called *forward δ -model* for $\beta = 0$ was used and γ operator is then

$$\gamma = \frac{z-1}{T_v} \quad (13)$$

The continuous model (11) is then rewritten to the form

$$a^\delta(\delta)y(t') = b^\delta(\delta)u(t') \quad (14)$$

where polynomials $a^\delta(\delta)$ and $b^\delta(\delta)$ are discrete polynomials and their coefficients are different from those of the CT model $a(s)$ and $b(s)$. Time t' is discrete time.

Now we can introduce substitution $t' = k - n$ for $k \geq n$ and Equation (14) then will be

$$\delta^2 y(k-n) = b_1^\delta \delta u(k-n) + b_0^\delta u(k-n) - a_1^\delta \delta y(k-n) - a_0^\delta y(k-n) \quad (15)$$

which means that the regression vector $\boldsymbol{\varphi}_\delta$ is then

$$\boldsymbol{\varphi}_\delta(k-1) = [-y_\delta(k-1), -y_\delta(k-2), u_\delta(k-1), u_\delta(k-2)]^T \quad (16)$$

and the vector of parameters $\boldsymbol{\theta}_\delta$ is generally

$$\boldsymbol{\theta}_\delta(k) = [a_1^\delta, a_0^\delta, b_1^\delta, b_0^\delta]^T \quad (17)$$

which is computed from the differential equation

$$y_\delta(k) = \boldsymbol{\theta}_\delta^T(k) \cdot \boldsymbol{\varphi}_\delta(k-1) + e(k) \quad (18)$$

where $e(k)$ is a general random immeasurable component.

3.1.2. Identification of ELM parameters

The Recursive Least-Squares (RLS) method is used for the parameter estimation in this work. The RLS method is well-known and widely used for the parameter estimation. It is usually modified with some kind of forgetting, exponential or directional. Parameters of the identified system can vary during the control which is typical for nonlinear systems and the use of some forgetting factor could result in better output response. The basic RLS method is described by the set of equations:

$$\begin{aligned} \varepsilon(k) &= y(k) - \boldsymbol{\varphi}_\delta^T(k) \cdot \hat{\boldsymbol{\theta}}_\delta(k-1) \\ \xi(k) &= [1 + \boldsymbol{\varphi}_\delta^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_\delta(k)]^{-1} \\ \mathbf{L}(k) &= \xi(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_\delta^T(k) \\ \mathbf{P}(k) &= \frac{1}{\lambda_1(k-1)} \left[\mathbf{P}(k-1) - \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_\delta(k) \cdot \boldsymbol{\varphi}_\delta^T(k) \cdot \mathbf{P}(k-1)}{\lambda_1(k-1) + \boldsymbol{\varphi}_\delta^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_\delta(k)} \right] \\ \hat{\boldsymbol{\theta}}_\delta(k) &= \hat{\boldsymbol{\theta}}_\delta(k-1) + \mathbf{L}(k) \varepsilon(k) \end{aligned} \quad (19)$$

RLS with the changing exp. forgetting is used for parameter estimation, where the changing forgetting factor λ_1 is computed from the equation

$$\lambda_1(k) = 1 - K \cdot \xi(k) \cdot \varepsilon^2(k) \quad (20)$$

where K is small number, in our case $K = 0.001$.

3.2. Dynamic Linear Part (DLP)

The DLP is constructed with the use of polynomial approach (Kucera 1993) similarly as it was used in adaptive control described in (Vojtesek et al. 2011).

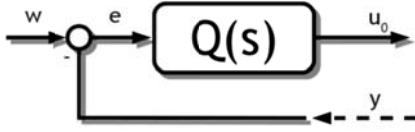


Figure 8: 1DOF control scheme in dynamic linear part

The control system configuration with one degree-of-freedom (1DOF) with controller in the feedback part was used here and it is displayed in Figure 8. The transfer function of the of the controller $Q(s)$ is designed with the use of polynomial synthesis:

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)} \quad (21)$$

where degrees of polynomials $\tilde{p}(s)$ and $q(s)$ are computed from:

$$\begin{aligned} \deg q(s) &= \deg a(s) + \deg f(s) - 1 \\ \deg \tilde{p}(s) &\geq \deg a(s) - 1 \end{aligned} \quad (22)$$

and parameters of these polynomials are computed by the Method of uncertain coefficients which compares coefficients of individual s -powers from the Diophantine equation, e.g. (Kucera 1993):

$$a(s) \cdot s \cdot \tilde{p}(s) + b(s) \cdot q(s) = d(s) \quad (23)$$

The polynomial $d(s)$ on the right side of (23) is an optional stable polynomial. It is obvious, that the degree of this polynomial is:

$$\deg d(s) = \deg a(s) + \deg \tilde{p}(s) + 1 \quad (24)$$

and roots of this polynomial are called poles of the closed-loop and their position affects quality of the control. This polynomial is designed via well-known Pole-placement method. A choice of roots needs some a priori information about the system's behavior. It is good to connect poles with the parameters of the system via spectral factorization. The polynomial $d(s)$ can be then rewritten to the form

$$d(s) = n(s) \cdot (s + \alpha)^{\deg d - \deg n} \quad (25)$$

where $\alpha > 0$ is an optional coefficient reflecting closed-loop poles and stable polynomial $n(s)$ is obtained from the spectral factorization of the polynomial $a(s)$

$$n^*(s) \cdot n(s) = a^*(s) \cdot a(s) \quad (26)$$

The Diophantine equation (23), as it is, is valid for step changes of the reference and disturbance signals which means that $\deg f(s) = 1$ in (22). This controller ensures stability, load disturbance attenuation and asymptotic tracking of the reference signal.

The order of the polynomials $q(s)$, $\tilde{p}(s)$ and $d(s)$ for second order transfer transfer function (11) are:

$$\begin{aligned} \deg q(s) &= \deg a(s) = 2 \\ \deg \tilde{p}(s) &\geq \deg a(s) - 1 \Rightarrow \deg \tilde{p}(s) = 1 \\ \deg d(s) &= \deg a(s) + \deg \tilde{p}(s) + 1 = 2 + 1 + 1 = 4 \end{aligned} \quad (27)$$

The transfer function of the controller is then

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s \cdot (s + p_0)} \quad (28)$$

and the polynomial $d(s)$ could be chosen as

$$d(s) = n(s) \cdot (s + \alpha)^2 \quad (29)$$

Parameters of the polynomial $n(s)$ which are computed from the spectral factorization are defined as:

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

The control system synthesis is done here in continuous time, but recursive identification uses discrete time steps. The resulted, so called "hybrid", controller works in the continuous time but parameters of the polynomials in the system's transfer function are identified recursively in the sampling period T_v . This assumption results in the condition, that the parameters of the δ -model are close the continuous ones for the small sampling period.

4. SIMULATION STUDIES

The proposed control strategy was tested on the mathematical model of the CSTR described in chapter 2. The goal was to test Due to comparability of the results, the common values for all simulations were: the sampling period was $T_v = 0.3 \text{ min}$, the simulation time 600 min and 6 different step changes were done during this time. The initial vector of parameters used for identification was $\hat{\theta}_s^T = [0.1, 0.1, 0.1, 0.1]$ and the initial covariance matrix was $P_{ii} = 1 \cdot 10^7$ for $i = 1, \dots, 4$. The simulation was done for the different values of the position of the root α in (29), $\alpha = 0.06, 0.12$ and 0.18 .

The first experiment simulates nonlinear adaptive control with ELM in the form of transfer function (11) and feedback 1DOF controller (28). Resulting courses of the reference signal (wanted value), $w(t)$, the input variable, $u(t)$, and the output variable $y(t)$ are shown in Figure 9 and Figure 10. Note, that the output variable $y(t)$ represents difference of the actual value of the

reactant's temperature from its steady-state value. This was done because we want the output to start from zero. On the other hand, the input variable $u(t)$ shows change of the volumetric flow rate of the coolant from its steady-state value. The input and output variables are then:

$$u(t) = q_c - q_c^s; y(t) = T(t) - T^s \quad (31)$$

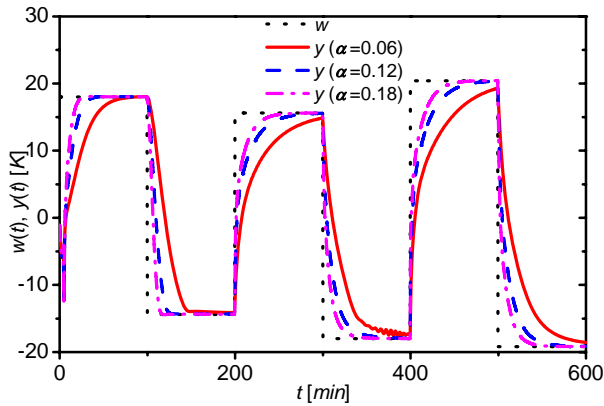


Figure 9: The course of the reference signal, $w(t)$, and the output variable, $y(t)$, for different values of the parameter α

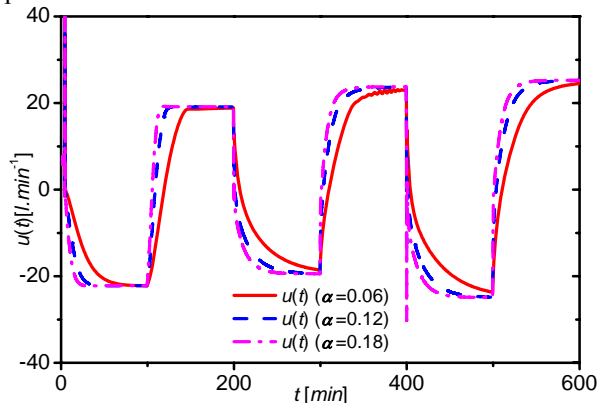


Figure 10: The course of the input variable, $y(t)$, for different values of the parameter α

Figure 9 shows that proposed controlled did not have any serious problems with the control of this nonlinear process. As it was mentioned, the control response could be tuned via choice of the parameter α in (29). It is clear, that the increasing value of this parameter results in quicker output response.

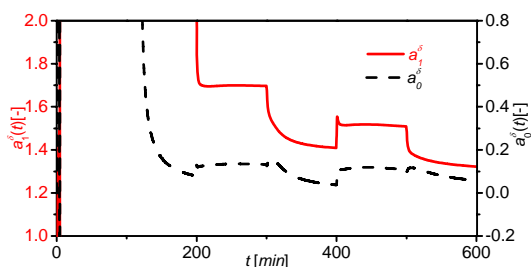


Figure 11: The course of the identified parameters a_1^δ and a_0^δ during the control for $\alpha = 0.12$

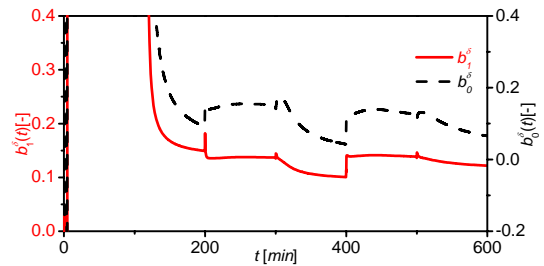


Figure 12: The course of the identified parameters b_1^δ and b_0^δ during the control for $\alpha = 0.12$

The course of the identified parameters a_1^δ , a_0^δ , b_1^δ and b_0^δ for parameter $\alpha = 0.12$ during the control is shown in Figure 11 and Figure 12.

It is obvious, that the controller needs some initial time, in our case about 150-200 min for adaptation. That is why the values are cut – the original values will rescale the graphs and devalue results. On the other hand, this adaptation does not influence results of control as it can be seen in Figure 9 and Figure 10.

The second analysis compares results of the nonlinear adaptive control with the ordinary adaptive control without the SNP. Courses of the output and input variables for the value of the parameter $\alpha = 0.12$ are shown in the following figures.

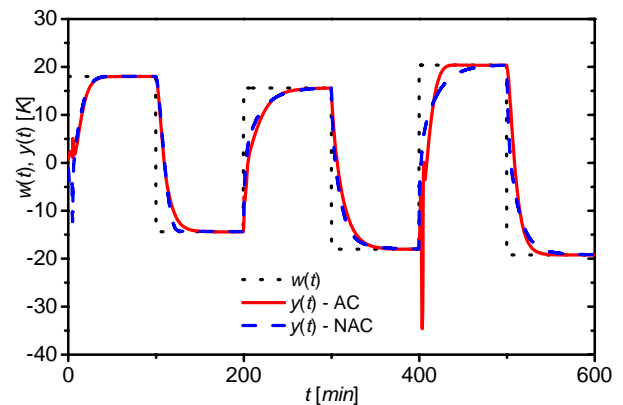


Figure 13: The course of the reference signal, $w(t)$, and the output variable, $y(t)$, for adaptive control (AC) and nonlinear adaptive control (NAC) for $\alpha = 0.12$

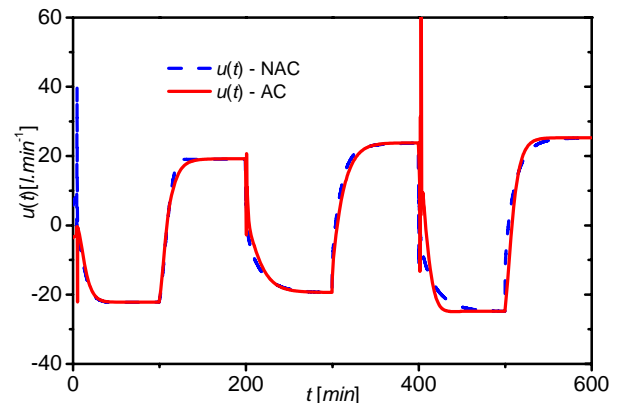


Figure 14: The course of the input variable, $u(t)$, for adaptive control (AC) and nonlinear adaptive control (NAC) for $\alpha = 0.12$

Presented results in Figure 13 and Figure 14 shows that the nonlinear adaptive control produces more stable and smooth course of both input and output variables than the ordinary adaptive control. This is evident at time $t = 400 \text{ min}$, when adaptive control produces very suboptimal output response and big changes of the input variable.

CONCLUSION

In this paper, the revised approach to the adaptive control with the static nonlinear part was used. The proposed control technique was tested by the simulation on the mathematical model of the continuous stirred tank reactor with the spiral cooling in the jacket as a typical member of the nonlinear system with lumped parameters. This mathematical model was described by the set of two ODE which were solved numerically. The nonlinear adaptive controller uses results of the steady-state analysis to help the controller to cope the nonlinearities. Used polynomial synthesis together with the pole-assignment method fulfills basic control requirements and moreover this controller could be tuned by the choice of the parameter α . Increasing value of this parameter results in quicker output response. The comparison with the pure adaptive control has shown usability of this method for bigger step changes of the reference signal. The controller could be also improved with the use of some predictive approach, for example Generalized Predictive Control (GPC) which will produce better control output. It will be part of our future work. We want to also test this control strategy by the control of the real plant or the real model of the plant which is necessary part of the verification.

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AUTHORS BIOGRAPHY

JIRI VOJTESEK was born in Zlin. Czech Republic and studied at the Tomas Bata University in Zlin. where he got his master degree in chemical and process engineering in 2002. He has finished his Ph.D. focused on Modern control methods for chemical reactors in 2007. His contact is vojtesek@fai.utb.cz.

PETR DOSTAL studied at the Technical University of Pardubice. He obtained his PhD. degree in Technical Cybernetics in 1979 and he became professor in Process Control in 2000. His research interest are modeling and simulation of continuous-time chemical processes. polynomial methods. optimal. adaptive and robust control. You can contact him on email address dostalp@fai.utb.cz.