Adaptive Control of Tubular Chemical Reactor

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Abstract: - In this paper the simulation results of the adaptive control inside the tubular chemical reactor with counter-current cooling in the jacket is shown. The adaptive controller is based on the choice of the External Linear Model as a linear representation of the originally nonlinear system parameters of which are identified recursively. The polynomial method together with spectral factorization and pole-placement method satisfies the basic control requirements. The controller could be tuned via position of the closed-loop root. Although the system has strongly nonlinear behaviour the proposed controller provides good control results.

Key-Words: - Tubular chemical reactor, Adaptive control, Recursive identification, Polynomial approach

1 Introduction

Tubular chemical reactor is tool frequently used in chemical industry for production of the several chemicals. From the mathematical point of view This type of reactor belongs to the class of systems with distributed parameters [1] from the mathematical point of view. Configuration with one main pipe with several pipes inside used in this work offers cooling in the remaining space of the main pipe with the same or opposite direction to the flow direction of the reactant. The direction of the cooling could be with the same direction as the flow of the reactant (co-current) or with the opposite direction (counter-current). It was proofed e.g. in [2], that the counter-current cooling used in this work has better cooling efficiency than co-current cooling.

Controlling of such processes with conventional methods with fixed parameters of the controller could be problem mainly in the cases where the working point changes. This inconvenience should be overcome with the use of some of "new" control strategies such as adaptive control, predictive control etc. This work show process of the designing of the adaptive controller [3]. The adaptation is process known from the animals and plants which adapts their behaviour to the environment. This process means the loss of the energy collects information and experiences about the system.

Adaptive approach here is based on the choice of the External Linear Model (ELM) of originally nonlinear system, parameters of which are estimate recursively and parameters of the controller are recomputed in each step according these identified ones.

The delta models [4] were used in ELM. Although these models belongs to the class of discrete-time models, parameters of such models approaches to the continuous-time ones for small sampling period [5].

The polynomial approach together with the pole-placement method [6] which are used for the designing of the controller satisfy basic control requirements such as stability, disturbance attenuation or reference signal tracking.

All simulations were done in the mathematical simulation software Matlab, version 6.5.

2 Nonlinear System

The nonlinear system under the consideration is represented by the tubular chemical reactor with simple exothermic reaction A $\rightarrow$ B $\rightarrow$ C [7]. Mathematical description of such process is very complex and so we introduce some simplifications. We neglect heat losses and conduction along the metal wall of the pipes, but heat transfer through the wall is consequential for a dynamic study. Furthermore, we expect that all densities, heat capacities and heat transfer coefficients are constant.

This type of chemical reactor provides two options for cooling from the direction point of view – (I.)co-current and (II.)counter-current cooling. It was proofed for example in [2], that the counter-current cooling has better cooling efficiency and that is why this type of cooling is used here. The

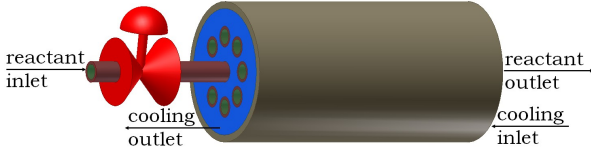graphical representation of the tubular chemical reactor can be found in Fig. 1.

Fig. 1 Tubular chemical reactor

2.1 Mathematical Model
The mathematical model is in this case described by the set of five PDE derived from the balances inside the reactor:

$$\frac{\partial c_A}{\partial t} + v_r \cdot \frac{\partial c_A}{\partial z} = -k_1 \cdot c_A \qquad (1)$$

$$\frac{\partial c_B}{\partial t} + v_r \cdot \frac{\partial c_B}{\partial z} = k_1 \cdot c_A - k_2 \cdot c_B \qquad (2)$$

$$\frac{\partial T_r}{\partial t} + v_r \cdot \frac{\partial T_r}{\partial z} = \frac{Q_r}{\rho_r \cdot c_{rp}} - \frac{4 \cdot U}{d_1 \cdot \rho_r \cdot c_{pr}} \cdot (T_r - T_w) \qquad (3)$$

$$\frac{\partial T_w}{\partial t} = \frac{4 \cdot [d_1 U_1 (T_r - T_w) + d_2 U_2 (T_c - T_w)]}{(d_2^2 + d_1^2) \cdot \rho_w \cdot c_{pw}} \qquad (4)$$

$$\frac{\partial T_c}{\partial t} - v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2 \cdot (T_w - T_c)}{(d_3^2 - n_1 \cdot d_2^2) \cdot \rho_c \cdot c_{pc}} \qquad (5)$$

where T is the temperature, d represents diameters, ρ are densities, c_p means specific heat capacities, U stands for the heat transfer coefficients, n_1 is a number of tubes and L represents the length of the reactor. Index $(\bullet)_r$ means the reaction compound, $(\bullet)_w$ is for the metal wall of the pipes and $(\bullet)_c$ for the cooling liquid. Variables v_r and v_c are fluid velocities of the reactant and cooling liquid, respectively, as

$$v_r = \frac{q_r}{f_r}; \quad v_c = \frac{q_c}{f_c} \qquad (6)$$

where q are flow rates and f are constants

$$f_r = n_1 \cdot \frac{\pi \cdot d_1^2}{4}; \quad f_c = \frac{\pi}{4} \cdot (d_3^2 - n_1 \cdot d_2^2) \qquad (7)$$

The reaction velocities, k_i, in equations (1) - (2) and equations are nonlinear functions of the temperature computed via the Arrhenius law:

$$k_j = k_{0j} \cdot \exp\frac{-E_j}{R \cdot T_r}, \text{ for } j = 1,2 \qquad (8)$$

where k_{0j} represents pre-exponential factors, E means activation energies and R is a gas constant. Q_r in the equation (3) is reaction heat computed as

$$Q_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B \qquad (9)$$

and h_j is used for reaction enthalpies.

The mathematical model shows that this plant is *a nonlinear system with continuously distributed parameters* [1]. Strong nonlinearity can be found in Equation (3), and the system is with distributed parameters because of the presence of the PDE where the state variable is related not only to the time variable, t, but the space variable, z, too.

In this case the initial conditions are $c_A(z,0) = c_A^s(z)$, $c_B(z,0) = c_B^s(z)$, $T_r(z,0) = T_r^s(z)$, $T_w(z,0) = T_w^s(z)$ and $T_c(z,0) = T_c^s(z)$ and boundary conditions $c_A(0,t) = c_{A0}(t)$, $c_B(0,t) = c_{B0}(t) = 0$, $T_r(0,t) = T_{r0}(t)$ and $T_c(L,t) = T_{cL}(t)$.

Fixed parameters of the reactor [7] are shown in the following Table 1:

$d_1 = 0.02\ m$	$c_{pc} = 4.18\ kJ.kg^{-1}.K^{-1}$
$d_2 = 0.024\ m$	$U_1 = 2.8\ kJ.m^{-2}.K^{-1}.s^{-1}$
$d_3 = 1\ m$	$U_2 = 2.56\ kJ.m^{-2}.K^{-1}.s^{-1}$
$n_1 = 1200$	$k_{10} = 5.61\times10^{16}\ s^{-1}$
$L = 6\ m$	$k_{20} = 1.128\times10^{16}\ s^{-1}$
$q_r = 0.15\ m^3.s^{-1}$	$E_1/R = 13477\ K$
$q_c = 0.275\ m^3.s^{-1}$	$E_2/R = 15290\ K$
$\rho_r = 985\ kg.m^3$	$h_1 = 5.8\times10^4\ kJ.kmol^{-1}$
$\rho_w = 7800\ kg.m^3$	$h_2 = 1.8\times10^4\ kJ.kmol^{-1}$
$\rho_c = 998\ kg.m^3$	$c_{A0}^s = 2.85\ kmol.m^{-3}$
$c_{pr} = 4.05\ kJ.kg^{-1}.K^{-1}$	$T_{r0}^s = 323\ K$
$c_{pw} = 0.71\ kJ.kg^{-1}.K^{-1}$	$T_{c0}^s = 293\ K$

Table 1: Fixed parameters of the reactor

2.2 Steady-state and Dynamic Analyses
The steady-state and dynamic analyses usually precede the design of the controller because they help with the understanding of the system's behaviour.

From the mathematical point of view, the static analysis means solving of the set of PDE (1) - (5) for the time close to infinity, which means that all derivatives with respect to time are equal to zero. The position derivatives can be replaced easily by the first forward differences, i.e.

$$\begin{aligned}\frac{dx}{dz}\bigg|_{z=z_0} &\approx \frac{x(i) - x(i-1)}{h_z} \\ \frac{dx}{dz}\bigg|_{z=z_0} &\approx \frac{x(j+1) - x(j)}{h_z}\end{aligned} \qquad (10)$$

where x is a general variable, h_z is an optional size of the step in axial direction, $i = 1, 2, \ldots, n$ and $j = n, n-1, \ldots, 0$. The defined input boundary conditions, x_0, for $i = 1$ are equal to boundary conditions $x(0)$. If the reactor is divided into N_z equivalent parts, the discretization step is

$$h_z = \frac{L}{N_z} \qquad (11)$$

where L denotes the length of the reactor and $N_z = 100$.

The steady-state analysis results in the working point which is in this case defined by the volumetric flow rate of the reactant $q_r^s = 0.150 \ m^3.s^{-1}$ and the volumetric flow rate of the coolant $q_c^s = 0.275 \ m^3.s^{-1}$.

The second, dynamic, analysis examines the behaviour after the step change of one of the input variables. Because the set of PDE (1) - (5) includes again derivatives with the respect to axial variable z, the discretization (11) must be used. The set of PDE is then transformed to a set of ODE which is then solved by the standard Runge-Kutta's method.

Although there are several input variables, the dynamic analysis here was done for different step changes of the volumetric flow rate of the cooling liquid, Δq_c^s. The output variable $y(t)$ illustrate the difference between the actual values of the reactive temperature, T_r, at the end of the reactor ($z = L$) and its steady-state value T_r^s. Mathematically speaking, there input and output variables are described as

$$u(t) = \frac{q_c(t) - q_c^s}{q_c^s} \cdot 100 \, [\%] \qquad (12)$$
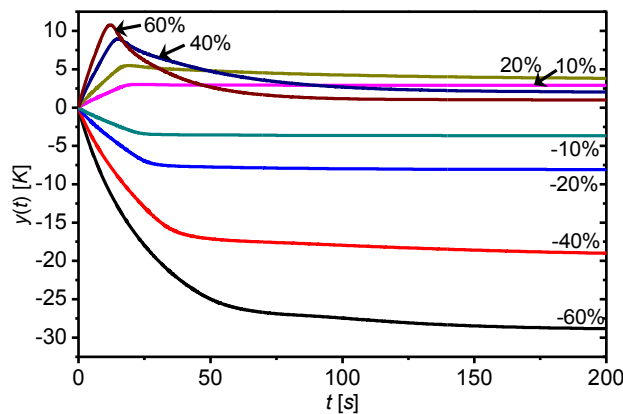
$$y(t) = T_r(t, L) - T_r^s \, [K]$$

Fig. 2: Output response to the step change of the input volumetric flow rate of the cooling, Δq_c

The output response displayed in Fig. 2 shows that this output should be expressed for example by second order transfer function with relative order one for the case of non-minimum phase behaviour:

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{a_2 s^2 + a_1 s + a_0} \qquad (13)$$

where the parameter a_2 is $a_2 = 1$ due to simplification.

3 Adaptive Control

The adaptive approach here is based on the recursive parameter identification of the ELM (13) which represents originally nonlinear system and parameters of the controller are recomputed according to the estimated parameters in every step too [3].

The controller is designed via polynomial synthesis [6] which fulfils basic control requirements and it can be used for systems with negative control properties. The control configuration with one degree-of-freedom (1DOF) is displayed in Fig. 3.
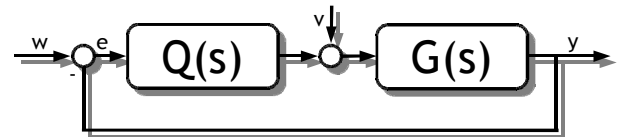

Fig. 3 1DOF control configuration

Block Q in Fig. 3 represents the transfer function of the controller, G denotes the transfer function (13) of the plant, w is the reference signal, e is used for the control error, v is the disturbance at the input to the system, u determines the input variable, and finally y is the output variable. Polynomials $a(s)$ and $b(s)$ in the transfer function (14) are commensurable polynomials in complex s-plane. The feasibility condition is fulfilled if the system is proper, i.e. deg $a(s) \geq$ deg $b(s)$.

The transfer function of the controller then is

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)} \qquad (14)$$

where polynomials $q(s)$ and $\tilde{p}(s)$ are computed from the Diophantine equation

$$a(s) \cdot s \cdot \tilde{p}(s) + b(s) \cdot q(s) = d(s) \qquad (15)$$

by the method of uncertain coefficients which compares coefficients of individual s-powers. The polynomial $d(s)$ on the right side of (15) is stable optional polynomial which fulfills the stability of the controller.

Degrees of the polynomials $q(s)$, a $\tilde{p}(s)$ and $d(s)$ are for the transfer function (14)

$$\deg \tilde{p}(s) \geq \deg a(s) - 1 = 1$$
$$\deg q(s) = \deg a(s) = 2 \qquad (16)$$
$$\deg d(s) = \deg a(s) + \deg \tilde{p}(s) + 1 = 4$$

which means that the transfer function of the controller in Equation (14) could be rewritten to form

$$\tilde{Q}(s) = \frac{q_2 s^2 + q_1 s + q_0}{s \cdot (p_1 s + p_0)} \qquad (17)$$

The optional polynomial $d(s)$ is in our case

$$d(s)=m(s) \cdot n(s) \qquad (18)$$

where $m(s)$ is $m(s)=(s+\alpha)^2$ for $\alpha > 0$ and $n(s)$ comes from the spectral factorization of $a(s)$:

$$n^*(s) \cdot n(s) = a^*(s) \cdot a(s)$$
$$n_0 = \sqrt{a_0^2} \qquad (19)$$
$$n_1 = \sqrt{a_1^2 + 2 n_0 - 2 a_0}$$

Polynomials $a(s)$ and $b(s)$ in (13), (15) and (19) are known from the recursive identification.

The delta (δ–) models were used for the estimation model. Although the delta models belong to the class of discrete-time models, parameters of such model approach to the continuous-time model for small sampling period [5].

The δ–model introduces a new complex variable γ computed as (see [4]):

$$\gamma = \frac{z-1}{\beta \cdot T_v \cdot z + (1-\beta) \cdot T_v} \qquad (20)$$

where β is a parameter from the interval $0 \le \beta \le 1$ and T_v means 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

$$\gamma = \frac{z-1}{T_v} \qquad (21)$$

The continuous model (13) is then rewritten to the form

$$a^\delta(\delta) y(t') = b^\delta(\delta) u(t') \qquad (22)$$

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 $b(s)$.

The transfer function $G(s)$ in (13) could be rewritten to the form of differential equation:

$$y_\delta(k) = -a_1^\delta y_\delta(k-1) - a_0^\delta y_\delta(k-2) + ... $$
$$+ b_1^\delta u_\delta(k-1) + b_0^\delta u_\delta(k-2) \qquad (23)$$

which is in the vector form

$$y_\delta = \theta_\delta^T(k) \cdot \varphi_\delta(k-1) \qquad (24)$$

and the vector of the parameters, θ_δ, and the data vector, φ_δ, are then

$$\theta_\delta(k) = \left[a_1^\delta, a_0^\delta, b_1^\delta, b_0^\delta \right]^T$$
$$\varphi_\delta(k-1) = \left[-y_\delta(k-1), -y_\delta(k-2) ... \right. \qquad (25)$$
$$\left. ..., u_\delta(k-1), u_\delta(k-2) \right]^T$$

$$y_\delta(k) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_v^2}$$
$$y_\delta(k-1) = \frac{y(k-1) - y(k-2)}{T_v}$$
$$y_\delta(k-2) = y(k-2) \qquad (26)$$
$$u_\delta(k-1) = \frac{u(k-1) - u(k-2)}{T_v}$$
$$u_\delta(k-2) = u(k-2)$$

The goal of the identification is to estimate vector of parameters θ_δ in ARX model (24) from the previous values of the input and output variables in the time intervals remote by sampling period T_v. The recursive least-squares method with exponential forgetting was used for identification in this work.

4 Simulation Results

All simulations were done for time $T_f = 10\,000$ s and five different step changes every 2 000 s were simulated during this time. The sampling period was $T_v = 1.5$ s and the controller was set to $\alpha = 0.007$, 0.01 and 0.02.
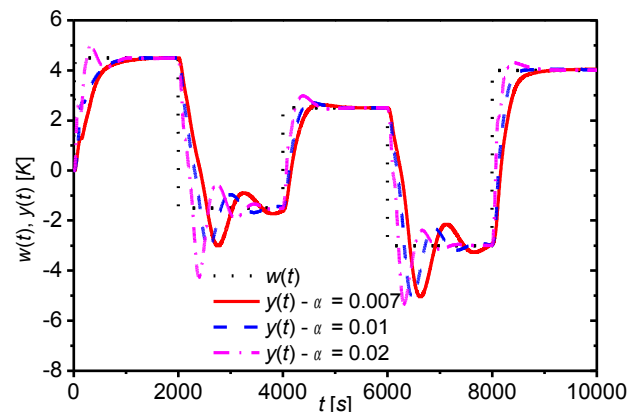

Fig. 4: The course of the output variable $y(t)$ for various α

Simulation results displayed in Fig. 4 and Fig. 5 clearly shows that the increasing value of the parameter α results in quicker output response but overshoots especially if the the value of the reference signal $w(t)$ jumps from the higher value to the lower one. Jumps from lower value to the higher has generally much better responses. The highest value of α, i.e. $\alpha = 0.021$ also generates much quicker and shaking changes of the input variable $u(t)$ (see Fig. 5) which is not very good from the practical point of view while this variable represents the twist of the valve and rapid changes could influence the vitality of the valve.
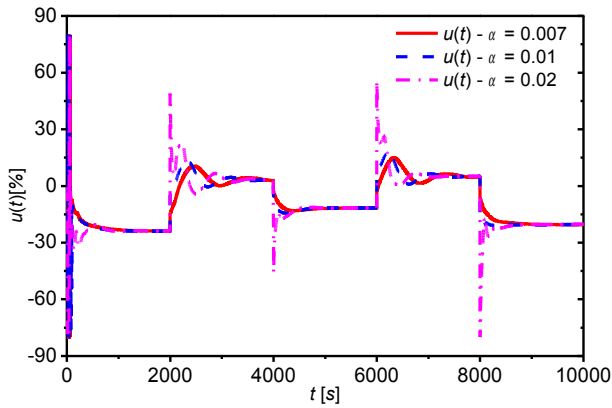
Fig. 5 The course of the input variable $u(t)$ for various α

The course of the identified parameters $a_1^\delta, a_0^\delta, b_1^\delta, b_0^\delta$ shown in Fig. 6 - 9 also shows usability of this control method. The only problem with the identification could be found at the very beginning of the control when the controller does not have enough information about the plant because the estimated vector starts from the general form $\theta_\delta(k) = [0.1, 0.1, 0.1, 0.1]^T$. On the other hand, the step changes does not provide such problems and estimation to the new variables is very quick.
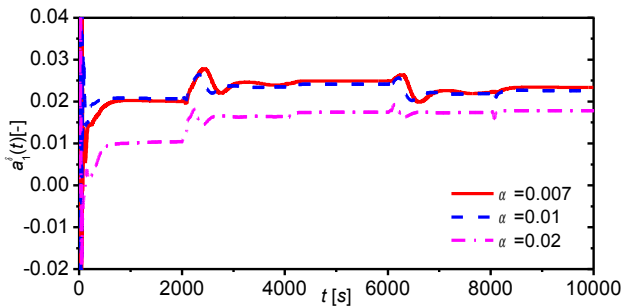

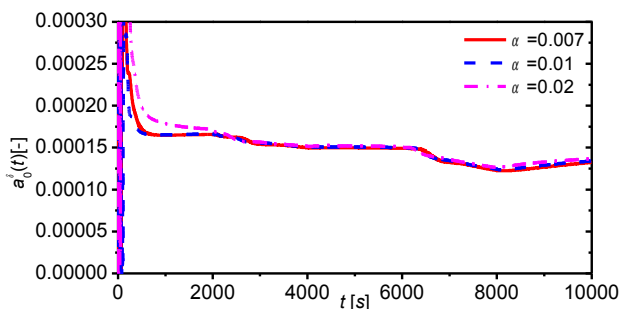Fig. 6 The course of the identified parameter a_1^δ for various α

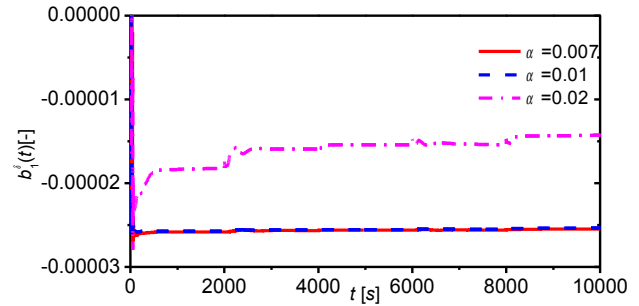Fig. 7 The course of the identified parameter a_0^δ for various α

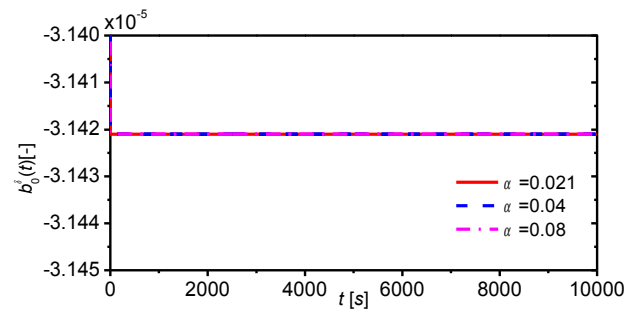Fig. 8 The course of the identified parameter b_1^δ for various α

Fig. 9 The course of the identified parameter b_0^δ for various α

The quality of the control is qualified with the control quality criteria S_u and S_y computed as

$$S_u = \sum_{i=St}^{N} \left(u(i) - u(i-1)\right)^2 [-]; \qquad \text{for } N = \frac{T_f}{T_v} \quad (27)$$
$$S_y = \sum_{i=St}^{N} \left(w(i) - y(i)\right)^2 [K^2];$$

where St is starting time of the computation which is in this case due to inaccurate identification at the very beginning after the second step change in time 2 000 s, i.e. $St = 2000/T_v$. The results for all three simulations are shown in Table.

	S_u [-]	S_y [K^2]
$\alpha = 0.007$	335	16 077
$\alpha = 0.01$	5 012	9 130
$\alpha = 0.02$	22 425	7 547

Table 2 Control quality criteria S_u and S_y

This table clearly shows, that the control configuration with $\alpha = 0.02$ has the best results from the output point of view (criterion S_y). On the other hand, the controller with $\alpha = 0.007$ has the best results for the input (S_u).

5 Conclusion

The goal of this contribution was to show suitable control approach for controlling of a nonlinear process represented by the tubular chemical reactor. This adaptive controller could be tuned via position of the root α and it was proofed that the increasing value of this parameter results in quicker output response but bigger overshoots.

Although this system has nonlinear behaviour, the proposed controller provides good control results and it can be used for controlling such processes. The next step should be verification on the real plant.

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