# ADAPTIVE CONTROL OF CHEMICAL REACTOR

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**Abstract:** This paper deals with the adaptive control of the nonlinear process represented by the continuous stirred tank reactor (CSTR). This chemical equipment is widely used in the chemical industry for production of various chemicals and drugs. Computer simulation which is used in this work has several advantages over the experint on the real model – it saves costs, reduces dangerousity and speed up experiments. The paper presents one approach to the control of the chemical reactor based on the choice of the external linear model (ELM) of the originally nonlinear process parameters of which are identified recursively and parameters of the controller are then adopt to these estimated ones. The polynomial approach together linear quadratic (LQ) approach used for the controller synthesis show good control results although the system has negative control properties.

**Keywords:** Adaptive control, polynomial synthesis, LQ approach, CSTR, recursive identification

## 1 INTRODUCTION

Most of the processes in the technical praxis have nonlinear properties and usage of the classical control strategies, where parameters of the controller are fixed, results in very limited results or non-optimal control for the nonlinear processes. This paper shows the simulation results of adaptive control of nonlinear lumped-parameters model represented by the Continuous Stirred Tank Reactor (CSTR) with so called van der Vusse reaction inside the reactor (Chen, *et al.*, 1995). The mathematical model of this reactor is described by the nonlinear set of ordinary differential equations.

The adaptive approach used here is based on the recursive identification of the External Linear Model (ELM) of the originally nonlinear process and the parameters of the controller are recomputed in each step according to identified ones too (Bobal, *et al*., 2005).

A polynomial approach used for the controller synthesis has satisfied control requirements and moreover, it could be used for systems with negative properties such as non-minimum phase behaviour or for processes with time delays. Connected with LQ control technique, it fulfills the requirements of stability, asymptotic tracking of the reference signal and compensation of disturbances (Kucera, 1993). Resulting controller is strictly proper.

The external delta models (Middleton and Goodwin, 1990) were used for parameter estimation of the nonlinear system. Although delta models belong to the range of discrete models, parameters of these models are equal to parameters of their continuous-time counterparts up to some assumptions (Stericker and Sinha, 1993). The recursive least-squares method with the exponential forgetting was used in the estimation part. Recursive Least Squares (RLS) methods without the forgetting, with the exponential forgetting and the directional forgetting (Fikar and Mikles, 1999) respectively were used in this case.

All proposed control strategies were verified by computations and simulations in mathematical software MATLAB, version 6.5.

## 2 CHEMICAL REACTOR

The chemical reactor under the consideration is Continuous Stirred Tank Reactor (CSTR). The reaction inside the reactor is called *van der Vusse* reaction can be described by the following reaction scheme (Chen, *et al*., 1995):

$$\begin{aligned} &A \xrightarrow{k_1} B \xrightarrow{k_2} C \\ &2A \xrightarrow{k_3} D \end{aligned} \tag{1}$$

The graphical scheme of this reactor can be seen in Figure 1.

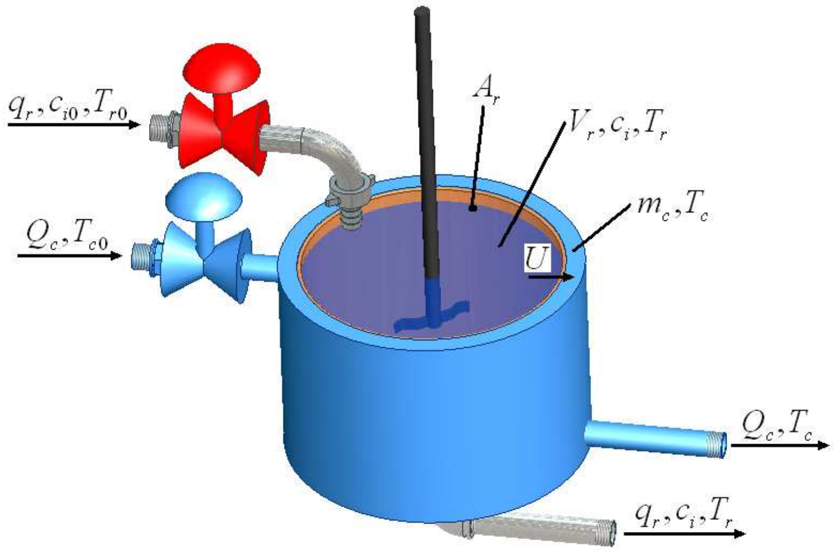


Figure 1: Continuous Stirred Tank Reactor (CSTR)

The mathematical model of this reactor is described by the following set of ordinary differential equations (ODE):

$$\begin{aligned} \frac{dc_A}{dt} &= \frac{q_r}{V_r}(c_{A0} - c_A) - k_1 c_A - k_3 c_A{}^2 \\ \frac{dc_B}{dt} &= -\frac{q_r}{V_r} c_B + k_1 c_A - k_2 c_B \\ \frac{dT_r}{dt} &= \frac{q_r}{V_r}(T_{r0} - T_r) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}}(T_c - T_r) \\ \frac{dT_c}{dt} &= \frac{1}{m_c c_{pc}}\left(Q_c + A_r U (T_r - T_c)\right) \end{aligned} \tag{2}$$

Table 1: Fixed parameters of the reactor

| | | |
|---|---|---|
| $k_{01} = 2.145 \cdot 10^{10}$ $min^{-1}$ | $k_{02} = 2.145 \cdot 10^{10}$ $min^{-1}$ | $k_{03} = 1.5072 \cdot 10^{8} min^{-1}.mol^{-1}$ |
| $E_1/R = 9758.3$ $K$ | $E_2/R = 9758.3$ $K$ | $E_3/R = 8560$ $K$ |
| $h_1 = -4200$ $kJ.kmol^{-1}$ | $h_2 = 11000$ $kJ.kmol^{-1}$ | $h_3 = 41850$ $kJ.kmol^{-1}$ |
| $V_r = 0.01$ $m^3$ | $m_c = 5$ $kg$ | $\rho_r = 934.2$ $kg.m^{-3}$ |
| $c_{pr} = 3.01$ $kJ.kg^{-1}.K^{-1}$ | $c_{pc} = 2.0$ $kJ.kg^{-1}.K^{-1}$ | $q_r = 2.365 \cdot 10^{-3}$ $m^3 min^{-1}$ |
| $c_{A0} = 5.1$ $kmol.m^{-3}$ | $c_{B0} = 0$ $kmol.m^{-3}$ | $T_{r0} = 387.05$ $K$ |
| $A_r = 0.215$ $m^2$ | $U = 67.2$ $kJ.min^{-1}m^{-2}K^{-1}$ | $Q_c = -18.5583$ $kJ.min^{-1}$ |

This set of ODE together with simplifications then mathematically represents examined CSTR reactor. The model of the reactor belongs to the class of *lumped-parameter nonlinear systems*. Fixed parameters of the system are shown in Table 1.

The reaction heat ($h_r$) in eq. (2) is expressed as:

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B + h_3 \cdot k_3 \cdot c_A^2 \qquad (3)$$

where $h_i$ means reaction enthalpies.

Nonlinearity can be found in reaction rates ($k_j$) which are described via Arrhenius law:

$$k_j\left(T_r\right) = k_{0j} \cdot \exp\left(\frac{-E_j}{RT_r}\right), \text{for } j = 1, 2, 3 \qquad (4)$$

where $k_0$ represent pre-exponential factors and $E$ are activation energies.

## 3 ADAPTIVE CONTROL

Adaptive control is one way to overcome problems with controlling of nonlinear systems. “Adaptivity” is derived from the living matters which adapts their behaviour and living to the behaviour of the neighbourhood. Each adaptation means loss of the energy and living matterms can minimize this loss with increasing number of continuous learning. This repetition is generally accumulation of the information. There are several types of adaptive systems described in (Bobal, *et al*., 2005). The adaptive approach used in our case is based on choosing of the External Linear Model (ELM) of the nonlinear process, parameters of which are estimated recursively and the parameters of the controller are then recomputed in every step according to estimated parameters of the ELM. The resulted controller works in continuous-time and in our case its structure corresponds to the structure of the real PID controller.

### 3.1 External Linear Model (ELM)

ELM as a presentation of a real system is usually described by continuous-time transfer function

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b(s)}{a(s)} \qquad (5)$$

where the condition of the properness is:

$$\deg b \le \deg a \qquad (6)$$

Polynomials $a(s)$, $b(s)$ can be generally expressed by

$$a(s) = \sum_{i=0}^{\deg a} a_i s^i, \; b(s) = \sum_{j=0}^{\deg b} b_j s^j \qquad (7)$$

And their coefficients $a_i$ and $b_j$ are estimated recursively during the control.

There can be used different types of ELM, e.g. continuous-time (CT) models (Vojtesek and Dostal, 2005), ordinary discrete models or $\delta$-models. There was used $\delta$-model as an ELM in this work. This model belongs to the class of discrete models but its properties are different according to the classical discrete model in Z-plain. If we want to convert Z-model to $\delta$–model, we must introduce a new complex variable $\gamma$ computed as (Mukhopadhyay, *et al*., 1992)

$$\gamma = \frac{z-1}{\alpha \cdot T_v \cdot z + (1-\alpha) \cdot T_v} \tag{8}$$

We can obtain infinitely many models for optional parameter $\alpha$ from interval $0 \le \alpha \le 1$, however *forward δ-model* were used in this work which has $\gamma$ operator computed via

$$\alpha = 0 \Rightarrow \gamma = \frac{z-1}{T_v} \tag{9}$$

ELM should be then generally described by equation

$$a'(\delta) y(t') = b'(\delta) u(t') \tag{10}$$

Where $t'$ denotes discrete time and $\delta$ is the operator. With decreasing value of the sampling period $T_v$ parameters of polynomials $a'(\delta)$ and $b'(\delta)$ approach to the parameters of the continuous-time model (5) (Stericker and Sinha, 1993).

Substitution $t' = k - n$ for $k \ge n$ in the equation (10) transfer this equation to

$$\begin{aligned} \delta^n y(k-n) &= b'_m \delta^m u(k-n) + \ldots + b'_1 \delta u(k-n) + b'_0 u(k-n) - \\ &- a'_{n-1} \delta^{n-1} y(k-n) - \ldots - a'_1 \delta y(k-n) - a'_0 y(k-n) \end{aligned} \tag{11}$$

And we can introduce simplification

$$\begin{aligned} & y_\delta(k) = \delta^n y(k-n), y_\delta(k-1) = \delta^{n-1} y(k-n), y_\delta(k-n+1) = \delta y(k-n), y_\delta(k-n) = y(k-n) \\ & u_\delta(k-n+m) = \delta^m u(k-n), u_\delta(k-n+1) = \delta u(k-n), u_\delta(k-n) = u(k-n) \end{aligned} \tag{12}$$

ARX (Auto-Regressive eXogenous) was used for identification. This model should be described by the differential equation

$$\hat{y}_\delta(k) = \boldsymbol{\theta}_\delta^T(k) \cdot \boldsymbol{\varphi}_\delta(k-1) + e(k) \tag{13}$$

Where $e(k)$ denotes immeasurable disturbances and $\boldsymbol{\varphi}_\delta$ is regression vector

$$\boldsymbol{\varphi}_\delta^T(k-1) = \left[-y_\delta(k-n), -y_\delta(k-n+1), \ldots, -y_\delta(k-1), u_\delta(k-n), u_\delta(k-n+1), \ldots, u_\delta(k-n+m)\right] \tag{14}$$

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

$$\boldsymbol{\theta}_\delta^T(k) = \left[a'_0, a'_1, \ldots, a'_{n-1}, b'_0, b'_1, \ldots, b'_m\right] \tag{15}$$

The most frequently used model is ARX model because it uses only directly measured quantities, predicted output $\hat{y}_\delta$ is only a function of measured data and simple *linear regression* should be used for parameter estimation.

## 3.2 Parameter estimation

As it is written above, adaptivity of the control process is fulfilled by the continuous parameter estimation during the control. Recursive Least Square (RLS) method was used for the parameter estimation. This method is well known and it does not need too much data storing during computation.

The recursive method used here for estimation is *RLS Method with Exponential Forgetting* which is modification of well known Ordinary recursive least-squares method (Fikar and Mikleš, 1999):.

$$
\begin{aligned}
\varepsilon(k) &= y(k) - \boldsymbol{\varphi}_{\delta}^{T}(k)\cdot\hat{\boldsymbol{\theta}}_{\delta}(k-1) \\
\gamma(k) &= \left[1 + \boldsymbol{\varphi}_{\delta}^{T}(k)\cdot\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}_{\delta}(k)\right]^{-1} \\
\mathsf{L}(k) &= \gamma(k)\cdot\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}_{\delta}(k) \\
\mathbf{P}(k) &= \mathbf{P}(k-1) - \gamma(k)\cdot\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}_{\delta}(k)\cdot\boldsymbol{\varphi}_{\delta}^{T}(k)\cdot\mathbf{P}(k-1) \\
\hat{\boldsymbol{\theta}}_{\delta}(k) &= \hat{\boldsymbol{\theta}}_{\delta}(k-1) + \boldsymbol{L}(k)\varepsilon(k)
\end{aligned}
\tag{16}
$$

Modifications are used mainly in the cases where parameters of the identified system can vary during the control which is typical for nonlinear systems. Exponential Forgetting is based on the modification of the covariance matrix **P** by the equation

$$
\mathbf{P}(k) = \frac{1}{\lambda_1(k-1)}\left[\mathbf{P}(k-1) - \frac{\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}_{\delta}(k)\cdot\boldsymbol{\varphi}_{\delta}^{T}(k)\cdot\mathbf{P}(k-1)}{\lambda_1(k-1) + \boldsymbol{\varphi}_{\delta}^{T}(k)\cdot\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}_{\delta}(k)}\right] \tag{17}
$$

Several types of exponential forgetting can be used, e.g. like RLS with constant exp. forgetting, RLS with increasing exp. forgetting etc. RLS with the changing exp. forgetting is used for parameter estimation, where the changing forgetting factor $\lambda_1$ is computed from the equation

$$
\lambda_1(k) = 1 - K\cdot\gamma(k)\cdot\varepsilon^2(k) \tag{18}
$$

Where $K$ is small number, e.g. $K = 0.001$.

## 3.3 Control System Configuration

There was used one degree-of-freedom configuration displayed in Figure 2 for designing of the controller.

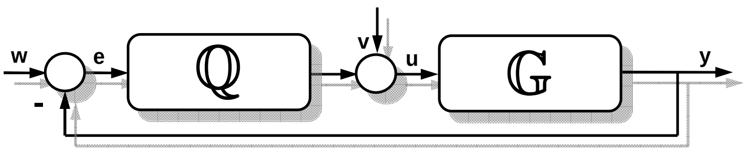


Figure 2: 1DOF control configuration

This control configuration has controller *Q* only in the feedback segment. *G* in Figure 2 denotes transfer function of controlled plant, *w* is the reference signal (wanted value), *v* is disturbance, *e* is used for control error, *u* is control variable and *y* is a controlled output.

Transfer functions of the controller (*Q*) is generally:

$$
Q(s) = \frac{q(s)}{s\cdot p(s)} \tag{19}
$$

where parameters of the polynomials $p(s)$ and $q(s)$ are computed from diophantine equation (Kucera, 1993):

$$
a(s)\cdot s\cdot p(s) + b(s)\cdot q(s) = d(s) \tag{20}
$$

Parameters of the polynomials $a(s)$ and $b(s)$ are known from the recursive identification and polynomial $d(s)$ is a stable polynomial. All these equations are valid for step changes of the reference and disturbance signals.

The controller $Q(s)$ ensures stability, load disturbance attenuation and asymptotic tracking for 1DOF configuration. A demand for a stable controller is fulfilled if the polynomial $p(s)$ in the denominator of (19) is stable. Inner properness holds if all transfer functions are proper. Transfer function $Q(s)$ in (19) is proper if

$$\deg q \leq \deg p + 1 \tag{21}$$

Degrees of the polynomials $p$ and $q$ are computed with respect to conditions (6), (21) and solvability of the diophantine equations (20) as follows

$$\deg q = \deg a, \deg p \geq \deg a - 1 \tag{22}$$

Roots of the polynomial $d(s)$ on the right side of the equations (20) are poles of the closed-loop and the control quality is determined by the placement of these poles. There are several ways for choosing of the polynomial $d(s)$ on the right side of equations (20). One approach is to choose $n$ different or multiple roots

$$d(s) = (s+\alpha)^m ; d(s) = (s+\alpha_1)^{m/2} \cdot (s+\alpha_2)^{m/2} \ldots \tag{23}$$

where $m$ is degree of the polynomial $d(s)$.

This method has one disadvantage, there is no rule how to choose roots $\alpha$. One way how to overcome this problem is to connect the choosing of the polynomial $d(s)$ with parameters of the controlled system. This can be done through spectral factorization (Vojtesek, *et al.*, 2004).

The third approach, which was used in our case combines spectral factorization and Linear Quadratic (LQ) tracking. The LQ approach is based on an optimal control theory and in addition to the basic control requirements it minimize the cost function in the complex domain

$$J = \frac{1}{2\pi j} \int_{-j\omega}^{j\omega} \left\{ E^*(s)\mu_w E(s) + \tilde{U}^*(s)\varphi_w \tilde{U}(s) \right\} ds \tag{24}$$

Where $\varphi_w > 0$ and $\mu_w \geq 0$ are weighting coefficients, $E(s)$ and $U(s)$ are transfer functions of the error and input variables respectively. The polynomial $d(s)$ is in this case

$$d(s) = g(s) \cdot n(s) \tag{25}$$

where polynomials $n(s)$ and $g(s)$ are computed from the spectral factorization

$$\begin{gathered} (a \cdot f)^* \cdot \varphi_w \cdot a \cdot f + b^* \cdot \mu_w \cdot b = g^* \cdot g \\ n^* \cdot n = a^* \cdot a \end{gathered} \tag{26}$$

where $f(s)$ is for the control variable $u(t)$ and disturbance $v(t)$ from the ring of step functions $f(s) = s$.

The resulted controller is strictly proper and the degree of the polynomial $d(s)$ is computed via

$$\deg d = \deg(g \cdot n) = 2 \deg a + 1 \tag{27}$$

# 4 SIMULATION RESULTS

## 4.1 Static and Dynamic Analyses

The steady-state analysis was done for various values of the input volumetric flow rate of the rectant, $q_r$, and various heat removal of the cooling liquid, $Q_c$.

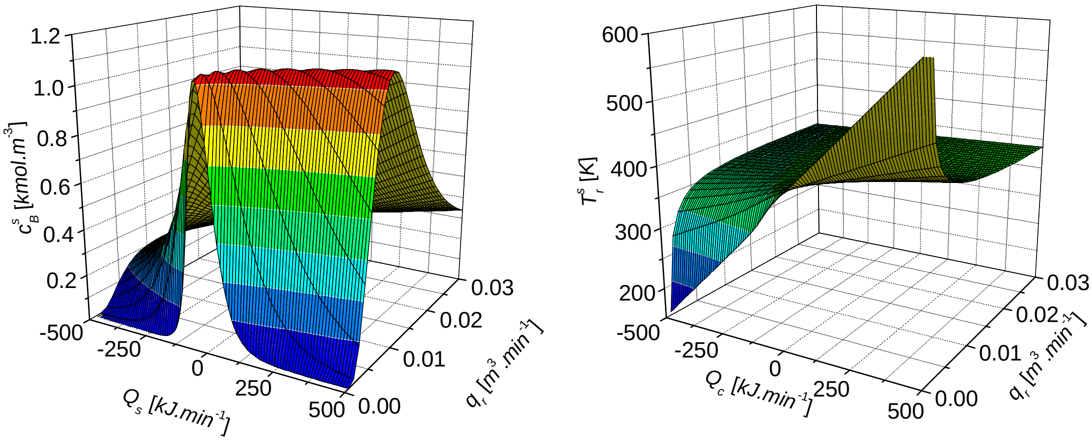


Figure 3: Steady-state values of the product's concentration, $c_B^s$, and the temperature of the reactant, $T_r^s$, for various heat removal, $Q_c$, and volumetric flow rate, $q_r$

3D-plots of the steady-state value of concentration $c_B^s$ and temperature $T_r^s$ presented in Figure 3 show high nonlinearity of the process. Static analysis usually results in an optimal working point. The maximum of the product's steady-state concentration, $c_B^s$, was chosen as a criterion for choosing an optimal working point. Concentration $c_B^s$ has its maximum for the volumetric flow rate $q_r^s = 2.365 \cdot 10^{-3}\ m^3.min^{-1}$ and the heat removal $Q_c^s = -18.56\ kJ.min^{-1}$.

The dynamic analysis was done for various step changes of the input heat removal of the cooling liquid, $Q_c$, and volumetric flow rate of the reactant, $q_r$. Four step changes ±10% and ±20% of both input variables – the heat removal $Q_c$ and the volumetric flow rate $q_r$ were done.

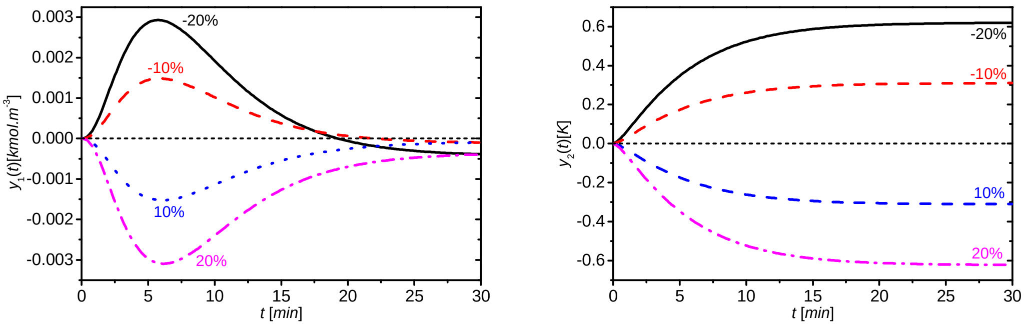


Figure 4: Dynamic analysis of outputs $y_1$ ($c_B(t) - c_B^s$) and $y_2$ ($T_r(t) - T_r^s$) for various step changes of the input heat removal, $Q_c$

The Figure 4 displays negative control properties of the system, especially for the first output $y_1$ which represents product's concentration $c_B$.

## 4.2 Adaptive control

The difference between actual and initial temperature of the reactant $T_r$ was taken as controlled output and changes of the heat removal $Q_c$ was set as control input, i.e.

$$\begin{aligned} y(t) &= T_r(t) - T_r^s(t)\,[K] \\ u(t) &= 100 \cdot \frac{Q_c(t) - Q_c^s(t)}{Q_c^s(t)}\,[\%] \end{aligned} \qquad (28)$$

On the other hand, dynamic analysis results in ELM represented by a second order transfer function with relative order one, which is generally:

$$G(s)=\frac{b(s)}{a(s)}=\frac{b_1 s+b_0}{s^2+a_1 s+a_0} \tag{29}$$

Equation (29) can be rewritten for the identification to the form of the differential equation

$$y_\delta(k)=-a_1 y_\delta(k-1)-a_0 y_\delta(k-2)+b_1 u_\delta(k-1)+b_0 u_\delta(k-2) \tag{30}$$

where $y_\delta$ is recomputed output to the $\delta$-model:

$$\begin{aligned} & y_\delta(k)=\frac{y(k)-2y(k-1)+y(k-2)}{T_v^2} \\ & y_\delta(k-1)=\frac{y(k-1)-y(k-2)}{T_v} \qquad u_\delta(k-1)=\frac{u(k-1)-u(k-2)}{T_v} \\ & y_\delta(k-2)=y(k-2) \qquad u_\delta(k-2)=u(k-2) \end{aligned} \tag{31}$$

where $T_v$ is the sampling period, the data vector is

$$\boldsymbol{\varphi}_\delta^T(k-1)=\left[-y_\delta(k-1),-y_\delta(k-2),u_\delta(k-1),u_\delta(k-2)\right] \tag{32}$$

and the vector of estimated parameters

$$\hat{\boldsymbol{\theta}}_\delta^T(k)=\left[\hat{a}_1',\hat{a}_0',\hat{b}_1',\hat{b}_0'\right] \tag{33}$$

could be computed from the ARX (Auto-Regressive eXogenous) model similar to(13):

$$y_\delta(k)=\hat{\boldsymbol{\theta}}_\delta^T(k)\boldsymbol{\varphi}_\delta(k-1) \tag{34}$$

by the recursive least squares methods described in part 3.2.

Degrees of the polynomials $p(s)$, $q(s)$ and $d(s)$ are then computed via (22) and (27):

$$\deg q=2;\ \deg p=2;\ \deg d=5 \tag{35}$$

Polynomials $g(s)$ and $n(s)$ in the equation (25) are

$$\begin{aligned} g(s)&=g_3 s^3+g_2 s^2+g_1 s+g_0 \\ n(s)&=s^2+n_1 s+n_0 \end{aligned} \tag{36}$$

and their coefficients are computed as

$$\begin{gathered} g_0=\sqrt{\mu_w b_0^2},\ g_1=\sqrt{2g_0 g_2+\varphi_w a_0^2+\mu_w b_1^2},\ g_2=\sqrt{2g_1 g_3+\varphi_w\left(a_1^2-2a_0\right)},\ g_3=\sqrt{\varphi_w}, \\ n_0=\sqrt{a_0^2},\ n_1=\sqrt{2n_0+a_1^2-2a_0} \end{gathered} \tag{37}$$

Transfer functions of the feedback and feedforward parts of the controller for 1DOF and 2DOF configurations are

$$Q(s)=\frac{q_2 s^2+q_1 s+q_0}{s\left(s^2+p_1 s+p_0\right)} \tag{38}$$

Where parameters of the polynomials $q(s)$ and $p(s)$ by the comparison of the coefficients of the $s$-powers a in diophantine equations (20).

All simulation experiments took 450 *min* and three changes were done during this interval. The first simulation study was done for various values of the weighting factor $\phi_w$ = 0.05, 0.5 and 1.5 in (37).

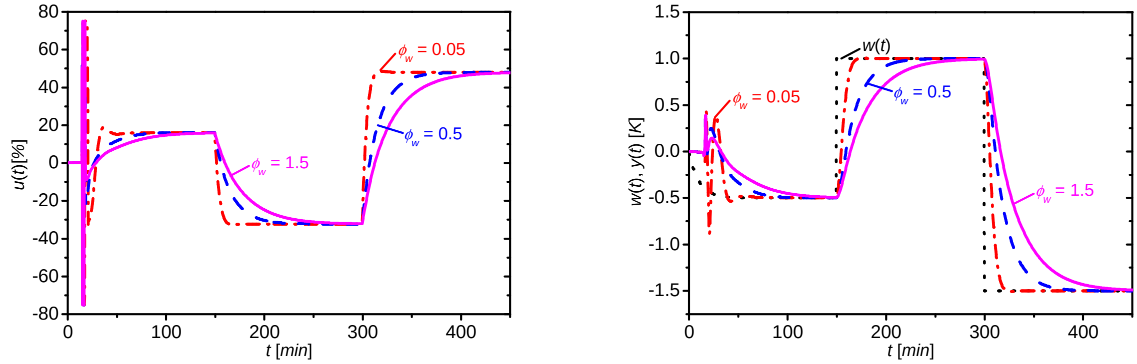


Figure 5: Course of input and output variables $u(t)$ and $y(t)$ for various weighting factors $\phi_w$, 1DOF configuration

As you can see in Figure 5, simulation is quicker with the decreasing value of the factor $\phi_w$. On the other hand, a low value of $\phi_w$ results in overshoots of the output response. There can be observed a few problems at the very beginning of the control. This is caused by the inaccurate parameter estimation which has a low amount of initial information about the system.

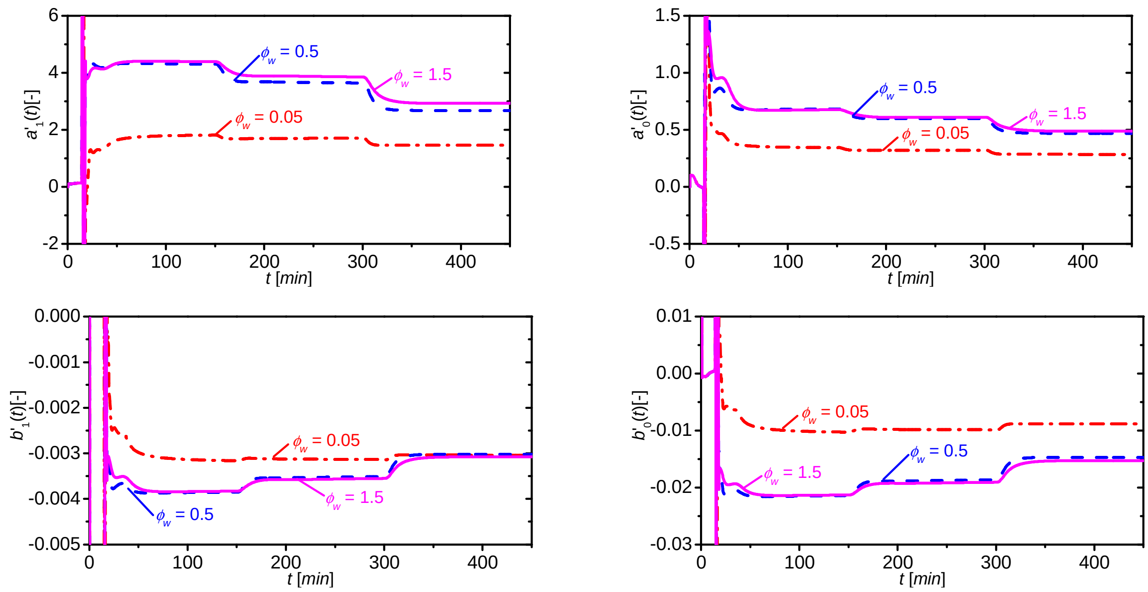


Figure 6: The course of identified parameters $a'_0$, $a'_1$, $b'_0$ and $b'_1$ during control, 1DOF, LQ method

Figure 6 shows the course of the identified parameters during the control. As you can see, used identification method has no significant problems except the begging of the control with is mentioned above.

## 5 CONCLUSION

This paper shows simulation results for adaptive control of a nonlinear lumped-parameters system represented by the CSTR reactor. Used adaptive control is based on the choosing of the external linear model in the range of delta models parameters of which are estimated recursively during the control. Three different recursive least squares methods were used for parameter estimation and two control system configurations with one degree-of-freedom (1DOF) and two degrees-of-freedom (2DOF). Presented results shows good control responses, the only problem is at the beginning of the control when we have less amount of information about the system. Course of the output temperature is quicker with the decreasing value of the weighting factor $\phi_w$ but there should be some small overshoots for low value of $\phi_w$. Comparison of 1DOF and 2DOF configurations presents slower course of the output variable for 2DOF but changes of the action value are smoother. The last analysis compares responses for different identifications and as it can be seen, there is no need for using forgetting factors because results are nearly the same.

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