HYBRID ADAPTIVE LQ CONTROL OF CHEMICAL REACTOR

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ABSTRACT

The paper shows one approach to control of a nonlinear process represented by an isothermal continuous stirred-tank reactor. The hybrid adaptive controller designed with the use of a polynomial synthesis, Linear-Quadratic approach and spectral factorization was used for controlling of the product‘s concentration via change of the volumetric flow rate of the reactant. An adaptivity of the system is satisfied by the on-line recursive identification of a external linear delta model of the system. The proposed control method satisfies basic control requirements such as a stability, a disturbance attenuation and a reference signal tracking. All methods are tested by the simulation on the mathematical software MATLAB.

INTRODUCTION

A major group of systems in the nature not only in the industry has a nonlinear behavior. The chemical rector is a typical member of nonlinear processes widely used in the chemical or the biochemical industry. The behavior of such processes could be observed by experiments on the real system or its smaller real model (Vojtesek and Dostal 2008). This method produce more realistic results but it could be dangerous or time and money demanding. The other approach uses modeling techniques for creating of a mathematical model as an abstract representation of the system. The mathematical model in the form of the set of Ordinary Differential Equations (ODE) is then subjected to simulations which show the static and the dynamic behavior of the system. The role of the simulation grows nowadays with the increasing speed and the decreasing price of computers.
The control of these processes with the conventional controllers with fixed parameters could lead to the unstable, inaccurate or unwanted output response when the state of the system change or the disturbance occurs. The adaptive control (Åström and Wittenmark 1989) is one way how we can solve these problems. This control method uses idea from the nature where plants or animals “adapt” their behavior to the actual state or environmental conditions. The adaptive controller adapts parameters or the structure to parameters of the controlled plant according to he selected criterion (Bobal et al. 2005).
The adaptive approach here is based on the choice of the External Linear Model (ELM) as a linear approximation of the originally nonlinear system, parameters of which are identified recursively and parameters of the controller are recomputed according to identified ones. The choice and the order of the ELM come from the dynamic analysis. The δ-models (Middleton and Goodwin 2004) used here are special type of discrete-time (DT) models parameters of which are related to the sampling period. It was proofed, that parameters of the δ-model approach to parameters of the continuous-time (CT) model for the small sampling period (Stericker and Sinha 1993).
The polynomial synthesis (Kucera 1993) together with the spectral factorization and the Linear-Quadratic (LQ) approach were used for designing of the controller. The product of this synthesis is the continuous-time controller which satisfies basic control requirements such as the stability, the reference signal tracking and the disturbance attenuation. The resulted controller is called “hybrid” because it works in continuous-time but its parameters are recomputed in discrete time intervals together with the δ-ELM identification.
The control technique was tested on the mathematical model of the isothermal Continuous Stirred-Tank Reactor (CSTR) the mathematical model of which is described by the set of five ordinary differential equations (Ingham et al. 2000).
All results shown in this contribution come from the simulation on the mathematical model and they were done on the mathematical simulation software Matlab.

ISOTHERMAL CHEMICAL REACTOR

The nonlinear system under the consideration is an isothermal Continuous Stirred-Tank Reactor (CSTR). The schematic representation of this reactor is in Figure 1. The reactions inside the reactor could be described by the scheme:

$$\begin{aligned} A + B &\xrightarrow{k_1} X \\ B + X &\xrightarrow{k_2} Y \\ B + Y &\xrightarrow{k_3} Z \end{aligned} \tag{1}$$

The must be introduced some simplifications to reduce the complexity of the system. First, as it is isothermal reactor, we expect that the temperature inside the reactor is constant during the reaction. We also assume

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constant volume of the reactor and perfect mixture of the reactant with the use the stirrer. The mathematical model of the system comes from the material balances inside the reactor together with all assumptions mentioned above.

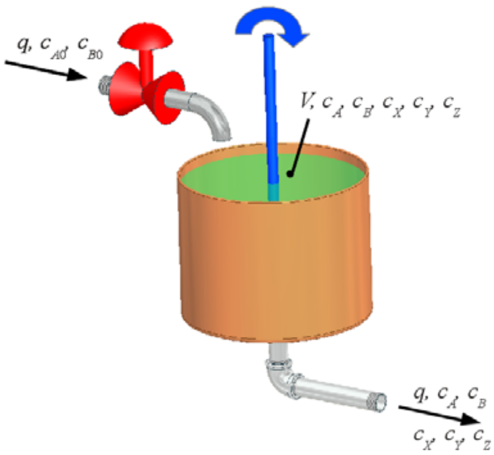

Figure 1: Isothermal Continuous Stirred-Tank Reactor

This model is then described by the set of Ordinary Differential Equations (ODEs) (Russell and Denn 1972):

$$
\begin{aligned}
\frac{dc_A}{dt} &= \frac{q}{V}\left(c_{A0}-c_A\right)-k_1\cdot c_A\cdot c_B\\
\frac{dc_B}{dt} &= \frac{q}{V}\left(c_{B0}-c_B\right)-k_1\cdot c_A\cdot c_B-\\
&\quad -k_2\cdot c_B\cdot c_X-k_3\cdot c_B\cdot c_Y\\
\frac{dc_X}{dt} &= \frac{q}{V}\left(c_{X0}-c_X\right)+k_1\cdot c_A\cdot c_B-k_2\cdot c_B\cdot c_X\\
\frac{dc_Y}{dt} &= \frac{q}{V}\left(c_{Y0}-c_Y\right)+k_2\cdot c_B\cdot c_X-k_3\cdot c_B\cdot c_Y\\
\frac{dc_Z}{dt} &= \frac{q}{V}\left(c_{Z0}-c_Z\right)+k_3\cdot c_B\cdot c_Y
\end{aligned}
\tag{2}
$$

where q denotes volumetric flow rate, V is used for volume of the reactant, c_A, c_B, c_X, c_Y and c_Z are concentrations, $k_{1\text{-}3}$ are rate constants and t is time. The fixed parameters are in Table 1 (Russell and Denn 1972).

Table 1: Fixed parameters of the reactor

Rate constants	$k_1 = 5\times10^{-4}\ m^3.kmol^{-1}.s^{-1}$ $k_2 = 5\times10^{-2}\ m^3.kmol^{-1}.s^{-1}$ $k_3 = 2\times10^{-2}\ m^3.kmol^{-1}.s^{-1}$
Input concentrations	$c_{A0} = 0.4\ kmol.m^{-3}$ $c_{B0} = 0.6\ kmol.m^{-3}$ $c_{X0} = c_{Y0} = c_{Z0} = 0\ kmol.m^{-3}$
Volume of the reactant	$V = 1\ m^3$

ADAPTIVE CONTROL

The control strategy here is based on the adaptive approach where the adaptivity is satisfied by the recursive identification of the External Linear Model (ELM) of the controlled nonlinear system.

The ELM comes from the static and dynamic analyses of the system. These analyses were discussed in detail in (Zelinka et al. 2006). If we choose the working point defined by the volumetric flow rate of the reactant $q^s = 1\times10^{-4}\ m^3.s^{-1}$, the steady-state values of the state variables in (2) are:

$$
\begin{aligned}
c_A^s &= 0.2407\ kmol.m^{-3} \qquad c_B^s = 0.1324\ kmol.m^{-3}\\
c_X^s &= 0.0024\ kmol.m^{-3} \qquad c_Y^s = 0.0057\ kmol.m^{-3}\\
c_Z^s &= 0.1513\ kmol.m^{-3}
\end{aligned}
\tag{3}
$$

Although there are six possible inputs to the system, such as a volumetric flow rate of the reactant q and input concentrations c_{A0}, c_{B0}, c_{X0}, c_{Y0} and c_{Z0}, from the control point of view only q could be used. Output concentrations of the product c_B was chosen as output variable. Variable y denote difference from their steady-state values, i.e.

$$y(t) = c_B(t) - c_B^s \tag{4}$$

It practically means that curves start from zero because these steady-state values are input conditions to the dynamic analysis. This helps better recognize of the gain of the system.

The results of six step changes ±100%, ±60% and ±30% of $q^s = 1\times10^{-4}\ m^3.s^{-1}$ are shown in following figure.

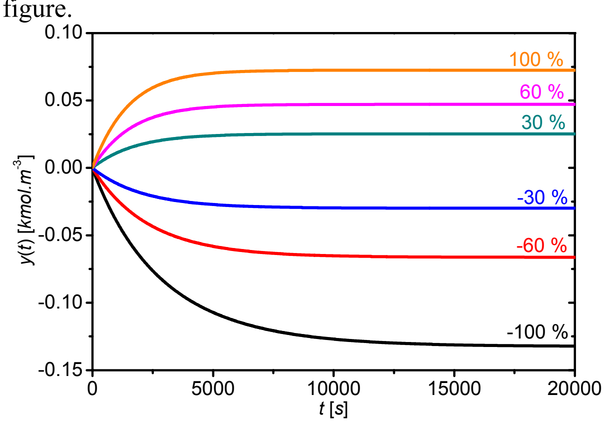

Figure 2: The course of the output concentration y_1 for the step changes of the volumetric flow rate q

External Linear Model (ELM)

Let us suppose, that the ELM of the controlled output displayed in Figure 2 could be described by the second order transfer function with relative order one in the s-plain, e.g.

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{a_2 s^2 + a_1 s + a_0} \tag{5}$$

where parameters of polynomials $a(s)$ and $b(s)$ are commensurable polynomials and the feasibility condition is fulfilled for $\deg a(s) \geq \deg b(s)$.

The transfer function is relation of the output from the system to the input which mathematically means that this continuous-time (CT) model (5) could be rewritten to:

$$a(\sigma)y(t) = b(\sigma)u(t) \tag{6}$$

where $a(\sigma)$ and $b(\sigma)$ are polynomials from (5) and σ is the differentiation operator. The identification of the CT model is not very simple. On the other hand, discrete-time(DT) identification could be inaccurate. Compromise between these two methods can be found in the use of so called Delta (δ-) models. This model uses a new complex variable γ defined generally as (Mukhopadhyay et al. 1992):

$$\gamma = \frac{z-1}{\beta \cdot T_v \cdot z + (1-\beta) \cdot T_v} \tag{7}$$

It is clear that we can obtain infinitely many models for the optional parameter β from the interval $0 \le \beta \le 1$ and a sampling period T_v. A forward δ-model was used in this work. The γ operator is then $\beta = 0 \rightarrow \gamma = (z-1)/T_v$ and the continuous model (6) could be then rewritten to

$$a^{\delta}(\delta)\, y(t') = b^{\delta}(\delta)\, u(t') \tag{8}$$

where polynomials $a^{\delta}(\delta)$ and $b^{\delta}(\delta)$ are discrete polynomials and their coefficients are different from those of the CT model $a(\sigma)$ and $b(\sigma)$. Time t' is the discrete time and with the new substitution $t' = k - n$ for $k \ge n$ the δ-model for this concrete transfer function would be:

$$\begin{aligned} \delta^2 y(k-n) &= b_1^{\delta} \delta u(k-n) + b_0^{\delta} u(k-n) - \\ &- a_1^{\delta} \delta y(k-n) - a_0^{\delta} y(k-n) \end{aligned} \tag{9}$$

The equation (9) produces both the regression vector $\boldsymbol{\varphi}_{\boldsymbol{\delta}}$ and the vector of parameters

$$\begin{aligned} \boldsymbol{\varphi}_{\boldsymbol{\delta}}(k-1) &= \left[-y_{\delta}(k-1), -y_{\delta}(k-2), u_{\delta}(k-1), u_{\delta}(k-2)\right]^T \\ \boldsymbol{\theta}_{\boldsymbol{\delta}}(k) &= \left[a_1^{\delta}, a_0^{\delta}, b_1^{\delta}, b_0^{\delta}\right]^T \end{aligned} \tag{10}$$

where y_{δ} and u_{δ} denotes the recomputed output and input variables to the δ-model and

$$\begin{aligned} y_{\delta}(k) &= \frac{y(k) - 2y(k-1) + y(k-2)}{T_v^2} \\ y_{\delta}(k-1) &= \frac{y(k-1) - y(k-2)}{T_v} \\ y_{\delta}(k-2) &= y(k-2) \\ u_{\delta}(k-1) &= \frac{u(k-1) - u(k-2)}{T_v} \\ u_{\delta}(k-2) &= u(k-2) \end{aligned} \tag{11}$$

The differential equation (9) has then the vector form:

$$y_{\delta}(k) = \boldsymbol{\theta}_{\boldsymbol{\delta}}^T(k) \cdot \boldsymbol{\varphi}_{\boldsymbol{\delta}}(k-1) + e(k) \tag{12}$$

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

On-line Identification

It is clear, that the unknown parameter from the differential equation (12) is the vector of parameters $\boldsymbol{\theta}_{\boldsymbol{\delta}}$. The regression vector $\boldsymbol{\varphi}_{\boldsymbol{\delta}}$ is constructed from the previous values of the measured inputs u and outputs y.
The Recursive Least-Squares (RLS) method is widely used for this on-line identification (Rao and Unbehauen 2005). This method is well-known and easily programmable. The RLS method with the changing exponential forgetting used here is described by the set of equations:

$$\begin{aligned} \varepsilon(k) &= y(k) - \boldsymbol{\varphi}_{\boldsymbol{\delta}}^T(k) \cdot \hat{\boldsymbol{\theta}}_{\boldsymbol{\delta}}(k-1) \\ \xi(k) &= \left[1 + \boldsymbol{\varphi}_{\boldsymbol{\delta}}^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_{\boldsymbol{\delta}}(k)\right]^{-1} \\ \boldsymbol{L}(k) &= \xi(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_{\boldsymbol{\delta}}^T(k) \\ \mathbf{P}(k) &= \frac{1}{\lambda_1(k-1)}\Bigg[\mathbf{P}(k-1) - \dots \\ &\dots - \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_{\boldsymbol{\delta}}(k) \cdot \boldsymbol{\varphi}_{\boldsymbol{\delta}}^T(k) \cdot \mathbf{P}(k-1)}{\lambda_1(k-1) + \boldsymbol{\varphi}_{\boldsymbol{\delta}}^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}_{\boldsymbol{\delta}}(k)}\Bigg] \\ \hat{\boldsymbol{\theta}}_{\boldsymbol{\delta}}(k) &= \hat{\boldsymbol{\theta}}_{\boldsymbol{\delta}}(k-1) + \boldsymbol{L}(k)\varepsilon(k) \end{aligned} \tag{13}$$

where the changing forgetting factor λ_1 is computed from the equation

$$\lambda_1(k) = 1 - K \cdot \xi(k) \cdot \varepsilon^2(k) \tag{14}$$

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

Design of Controller

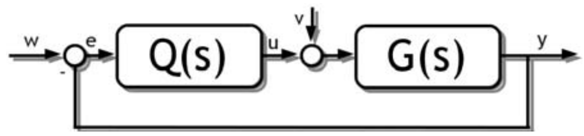

Figure 3: 1DOF control scheme

We can now introduce one simple feedback controller – see Figure 3, where $G(s)$ represents the transfer function (5) of the controlled output and $Q(s)$ denotes the transfer function of the controller in the continuous-time, generally:

$$Q(s) = \frac{q(s)}{p(s)} \tag{15}$$

where $q(s)$ and $p(s)$ are again commensurable polynomials with the properness condition $\deg p(s) \ge \deg q(s)$.
The Laplace transform of the transfer function $G(s)$ in (5) is

$$G(s) = \frac{Y(s)}{U(s)} \Rightarrow Y(s) = G(s) \cdot U(s) \tag{16}$$

where Laplace transform of the input signal u is from Figure 3

$$U(s) = Q(s) \cdot E(s) + V(s) = Q(s) \cdot \left[W(s) - Y(s)\right] + V(s) \tag{17}$$

If we put polynomials $a(s)$, $b(s)$, $p(s)$ and $q(s)$ into (17) instead of Laplace transforms $G(s)$ and $Q(s)$, the equation (16) has form

$$\begin{aligned} Y(s) &= \frac{b(s)q(s)}{a(s)p(s) + b(s)q(s)} \cdot W(s) + \dots \\ &\dots + \frac{a(s)p(s)}{a(s)p(s) + b(s)q(s)} \cdot V(s) \end{aligned} \tag{18}$$

and as you can see, both fractions has the same denominators which are called a characteristic polynomial of the closed loop and this polynomial can be rewritten to the form

$$a(s)\cdot p(s)+b(s)\cdot q(s)=d(s) \qquad (19)$$

where $d(s)$ is a stable optional polynomial and the whole equation (19) is called Diophantine equation (Kucera 1993). The stability of the control system is fulfilled for the stable polynomial $d(s)$ on the left side of the Diophantine equation (19). Asymptotic tracking of the reference signal and disturbance attenuation is attained if the polynomial $p(s)$ includes the least common divisor of denominators of transfer functions of the reference w and disturbance v:

$$p(s)=f(s)\cdot\tilde{p}(s) \qquad (20)$$

If we expect both these signals from the range of the step functions, the polynomial $f(s) = s$. The Diophantine equation (19) is then

$$a(s)\cdot s\cdot\tilde{p}(s)+b(s)\cdot q(s)=d(s) \qquad (21)$$

and the transfer function of the feedback controller is

$$\tilde{Q}(s)=\frac{q(s)}{s\cdot\tilde{p}(s)} \qquad (22)$$

As it is written above, the polynomial $d(s)$ on the right side of the Diophantine equation (21) is the stable optional polynomial. There are several ways how we can construct this polynomial. The simples one is the based on pole-placement method where $d(s)$ is divided into one or more parts with double, triple, etc. roots, e.g.

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

where $\alpha > 0$. The disadvantage of this method can be found in the uncertainty. There is no general rule which can help us with the choice of roots which are, of course, different for different controlled processes. One way how we can overcome this unpleasant feature is to use spectral factorization. Big advantage of this method is that it can make stable roots from every polynomial, even if it is unstable. The polynomial $d(s)$ is in this case

$$d(s)=n(s)\cdot g(s) \qquad (24)$$

where parameters of the polynomial $n(s)$ are computed from the spectral factorization of the polynomial $a(s)$ in the denominator of (5), i.e.

$$n^*(s)\cdot n(s)=a^*(s)\cdot a(s) \qquad (25)$$

The second part, polynomial $g(s)$, is computed with the use of the Linear Quadratic (LQ) tracking (Hunt at al. 1992) which is based on the minimizing of the cost function in the complex domain

$$J_{LQ}=\int_0^\infty\left\{\mu_{LQ}\cdot e^2(t)+\varphi_{LQ}\cdot\dot{u}^2(t)\right\}dt \qquad (26)$$

where $\varphi_{LQ} > 0$ and $\mu_{LQ} \geq 0$ are weighting coefficients, $e(t)$ is the control error and $\dot{u}(t)$ denotes the difference of the input variable. It practically means, that parameters of the polynomial $g(s)$ are computed from the spectral factorization

$$(a(s)\cdot f(s))^*\cdot\varphi_{LQ}\cdot a(s)\cdot f(s)+b^*(s)\cdot\mu_{LQ}\cdot b(s)=\ldots$$
$$\ldots=g^*(s)\cdot g(s) \qquad (27)$$

Degrees of unknown polynomials $\tilde{p}(s)$, $q(s)$ and $d(s)$ are for the fulfilled properness condition generally:

$$\begin{aligned}&\deg\tilde{p}(s)\geq\deg a(s)-1\\&\deg q(s)=\deg a(s)+\deg f(s)-1\\&\deg d(s)=2\deg a+1\\&\deg n(s)=\deg a(s)\\&\deg g(s)=\deg d(s)-\deg n(s)\end{aligned} \qquad (28)$$

and these degrees and polynomials are for our concrete second order transfer function in (5)

$$\begin{aligned}&\deg\tilde{p}(s)=2\Rightarrow\tilde{p}(s)=s^2+p_1s+p_0\\&\deg q(s)=2\Rightarrow q(s)=q_2s^2+q_1s+q_0\\&\deg d(s)=2\deg a+1=2\cdot2+1=5\\&\deg n(s)=2\Rightarrow n(s)=s^2+n_1s+n_0\\&\deg g(s)=3\Rightarrow g(s)=s^3+g_2s^2+g_1s+g_0\end{aligned} \qquad (29)$$

Polynomials $n(s)$ and $g(s)$ are computed as a results of spectral factorizations (25) and (27):

$$\begin{aligned}&g_0=\sqrt{\mu_{LQ}b_0^2},\ g_1=\sqrt{2g_0g_2+\varphi_{LQ}a_0^2+\mu b_1^2},\\&g_2=\sqrt{2g_1g_3+\varphi_{LQ}\left(a_1^2-2a_0\right)},g_3=\sqrt{\varphi_{LQ}},\\&n_0=\sqrt{a_0^2},n_1=\sqrt{2n_0+a_1^2-2a_0}\end{aligned} \qquad (30)$$

Polynomials $a(s)$ and $b(s)$ of the ELM are known from the recursive identification described in previous parts.

The goal of the control strategy is to find parameters of polynomials $\tilde{p}(s)$ and $q(s)$. The method of uncertain coefficients which compares coefficients of individual s-powers can be used for formulating of these coefficients. The transfer function of the controller (22) has than CT form:

$$\tilde{Q}(s)=\frac{q(s)}{s\cdot\tilde{p}(s)}=\frac{q_2s^2+q_1s+q_0}{s\cdot\left(s^2+p_1s+p_0\right)} \qquad (31)$$

This transfer function could be then transformed to the differential equation which is easily solvable with the use of numerical methods.

The final controller is called "hybrid" because the control input is computed in the continuous time but the identification of the ELM runs in the discrete time with the use of δ-models.

SIMULATION RESULTS

The proposed hybrid adaptive LQ controller was tested on the mathematical model of CSTR described above. Three simulation experiments were done. The first and the second compares influence of weighting factors φ_{LQ} and μ_{LQ} respectively and the third simulation observes impact of disturbances to the control of the system.

The controlled output was difference of the product's B concentration c_B from its steady-state value and the input variable was the change of the volumetric flow rate from it's steady-state value in percent for all simulations, i.e.

$$\begin{aligned} y(t) &= c_B(t) - c_B^s \left[kmol.m^{-3}\right] \\ u(t) &= \frac{q(t)-q^s}{q^s}\cdot 100\,[\%] \end{aligned} \tag{32}$$

The simulation time was set to 15 000 s, the sampling period was T_v = 10 s. The input variable $u(t)$ was limited inside the bounds <-100%; 100%>.

The first study sets factor μ_{LQ} = 0.5 and the second factor was set to φ_{LQ} = 4×10^{-5}; 8×10^{-4} and 5×10^{-3}. Six different step changes were done during the control and results are shown in Figure 4 and Figure 5.

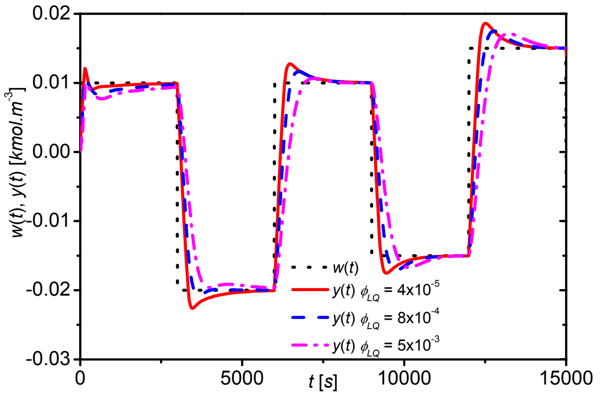

Figure 4: The course of the reference signal $w(t)$ and output responses $y(t)$ for different values of weighting factor φ_{LQ}

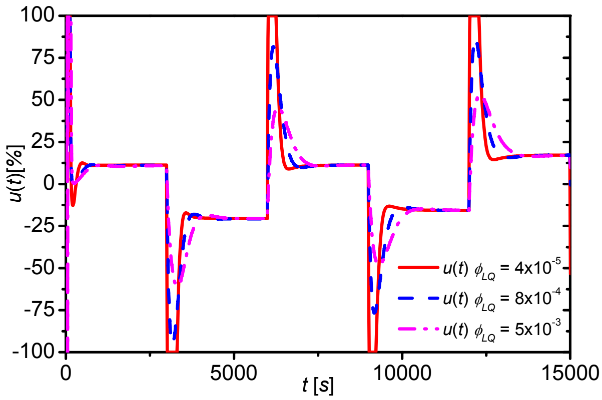

Figure 5: The course of the input signal $u(t)$ for different values of weighting factor φ_{LQ}

The results of the first study shows that the value of the weighting factor φ_{LQ} affects mainly the speed of the control. The increasing value of this factor produces slower course of the output variable $y(t)$ without overshoots – see Figure 4 and smoother course of the input variable $u(t)$ in Figure 5.

The second study was done for different values of the weighting factor μ_{LQ} = 0.5; 2 and 10 and a fixed value of the second weighting factor φ_{LQ} = 0.05. The same step changes as in the previous case were done and results are shown in Figure 6 and Figure 7.

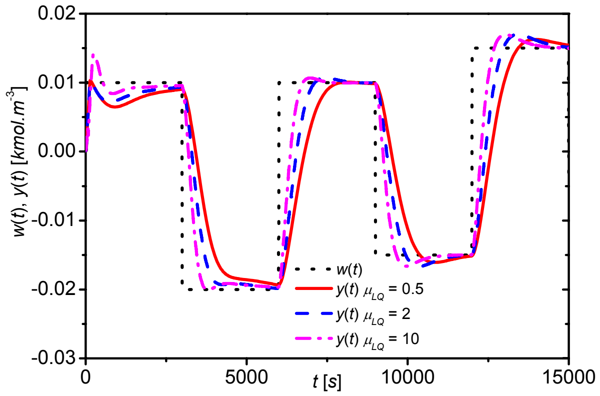

Figure 6: The course of the reference signal $w(t)$ and output responses $y(t)$ for different values of weighting factor μ_{LQ}

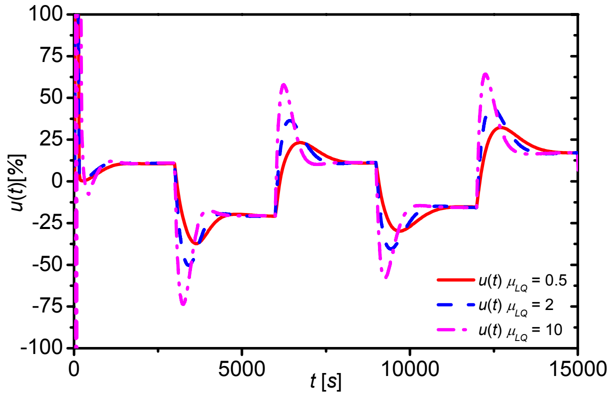

Figure 7: The course of the input signal $u(t)$ for different values of weighting factor μ_{LQ}

The affect of the weighting factor μ_{LQ} presented in previous graphs is opposite to the previous simulation study – increasing value of μ_{LQ} makes the course of the output variable $y(t)$ quicker but with small overshoots which depends on the change of the reference signal $w(t)$. Bigger change of $w(t)$ results in bigger overshoot and vice versa.

The only problem of both simulation studies can be found at the very beginning of the control where the course of the input variable and of course the output variable is very inaccurate. This is caused by the recursive identification which purposely starts from the general point $\boldsymbol{\theta}_\delta(0) = [0.1, 0.1, 0.1, 0.1]^T$ and it takes time 50-100 s to get the right vector of parameters.

The goal of the last simulation study is to show how this controller cope with the disturbances. Weighting factors were set to μ_{LQ} = 5; φ_{LQ} = 5×10^{-4} and two disturbances were injected into the system. The first disturbance was on the input concentration c_{B0}, $v_1(t)$ = -10% of c_{B0} for $t \in \langle 5000; 15000 \rangle\, s$ and the second disturbance on the output concentration c_B, $v_2(t)$ = +20% of c_B, was injected for the time $t \in \langle 10000; 15000 \rangle\, s$. The results are in the following figures.

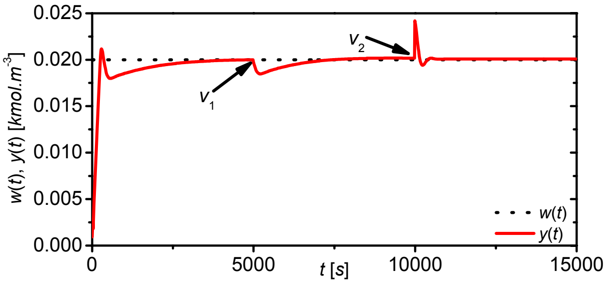

Figure 8: The influence of disturbances $v_1(t)$ and $v_2(t)$ to the output variable $y(t)$

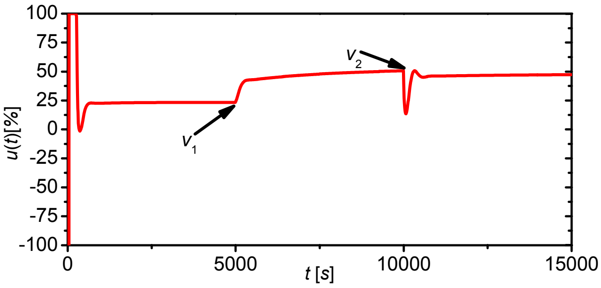

Figure 9: The influence of disturbances $v_1(t)$ and $v_2(t)$ to the input variable $y(t)$

Obtained results have shown, that proposed controller cope with both these disturbances without major problems even though both of these disturbences affects the system during simulation time $t \in \langle 10000;15000 \rangle s$.

CONCLUSION

The contribution shows one approach for controlling of the nonlinear process with lumped parameters represented by the isothermal CSTR. The hybrid controller was defined in the continuous-time but recursive identification uses discrete-time model based on the δ-model theory. The LQ approach together with the spectral factorization provides good control results although the system has nonlinear properties. The controller could be tuned with the choice of weighting factors φ_{LQ} or μ_{LQ}. Affect of both weighting factors was discussed in the practical simulation part. The value of these factors influence mainly the speed of the control and overshoots. This control strategy could be used also for similar types of nonlinear processes such as bath reactors, stirred reactor, tubular reactors, heat exchangers etc.

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