THE CONTINOUS STIRRED TANK REACTOR: ADAPTIVE LQ CONTROL

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Abstract: This paper deals with adaptive control of the Continuous Stirred Tank Reactor (CSTR) which is a typical member of nonlinear processes with lumped parameters. Since the controller is an adaptive one, parameters of the controller are estimated recursively during the control with different recursive least squares methods. 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 nonlinearity, non-minimum phase etc. Delta models were used as a external linear model of the nonlinear process. There were used two control configurations with one and two degrees-of-freedom for controller design. *Copyright* © *IFAC 2007*

Keywords: Adaptive LQ Control, CSTR, Recursive Identification, Delta Models, 1DOF and 2DOF Control Configurations

1. INTRODUCTION

Most of the processes in the technical praxis has nonlinear properties and usage of the classical control strategies, where parameters of the controller are fixed, results in very limited results or nonoptimal 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). Static analysis presented in (Vojtesek, *et al.*, 2004) have shown high nonlinearity of this process in the steady-state. On the other hand, dynamic analysis results in choosing of an External Linear Model (ELM).

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). Various types of identifications were 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.

Two control configurations were considered - one degree-of-freedom (1DOF) configuration which has controller only in the feedback part and two degrees-of-freedom (2DOF) configuration with feedback and feedforward parts (Grimble 1994).

All proposed control strategies were verified by computations and simulations in mathematical software MATLAB, version 6.5. The simulation results can demonstrate suitability of this control Next step should be verification on a real model.

2. 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.

2.1 External Linear Model (ELM)

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

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b(s)}{a(s)} \tag{1}$$

(2)

where the condition of the properness is: $\deg b \leq \deg a$

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

$$a(s) = \sum_{i=0}^{\deg a} a_i s^i, b(s) = \sum_{j=0}^{\deg b} b_j s^j$$
(3)

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 δ -models. There was used δ -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 δ -model, we must introduce a new complex variable γ computed as (Mukhopadhyay, *et al.*, 1992)

$$\gamma = \frac{z - 1}{\alpha \cdot T_{\nu} \cdot z + (1 - \alpha) \cdot T_{\nu}} \tag{4}$$

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

$$\alpha = 0 \Longrightarrow \gamma = \frac{z - 1}{T_{\nu}} \tag{5}$$

ELM should be then generally described by equation $a'(\delta) y(t') = b'(\delta)u(t')$ (6) Where t' denotes discrete time and δ is the operator. With decreasing value of the sampling period T_{ν} parameters of polynomials $a'(\delta)$ and $b'(\delta)$ approach to the parameters of the continuous-time model (1) (Stericker and Sinha, 1993).

Substitution t' = k - n for $k \ge n$ in the equation (6) transfer this equation to

$$\delta^{n} y(k-n) = b'_{m} \delta^{m} u(k-n) + \dots + b'_{1} \delta u(k-n) + b'_{0} u(k-n) - (7)$$

- $a'_{n-1} \delta^{n-1} y(k-n) - \dots - a'_{1} \delta y(k-n) - a'_{0} y(k-n)$
And we can introduce simplification

$$y_{\delta}(k) = \delta^{m} y(k-n), y_{\delta}(k-1) = \delta^{m} y(k-n), \dots$$

..., $y_{\delta}(k-n+1) = \delta y(k-n), y_{\delta}(k-n) = y(k-n)$
 $u_{\delta}(k-n+m) = \delta^{m} u(k-n), \dots$ (8)

$$\dots, u_{\delta}(k-n+1) = \delta u(k-n), u_{\delta}(k-n) = u(k-n)$$

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

$$\hat{y}_{\delta}(k) = \boldsymbol{\theta}_{\delta}^{T}(k) \cdot \boldsymbol{\varphi}_{\delta}(k-1) + e(k)$$
(9)

Where e(k) denotes immeasurable disturbances and φ_{δ} is regression vector

$$\boldsymbol{\varphi}_{\delta}^{T}(k-1) = \left[-y_{\delta}(k-n), -y_{\delta}(k-n+1), ..., -y_{\delta}(k-1), ... \\ ... u_{\delta}(k-n), u_{\delta}(k-n+1), ..., u_{\delta}(k-n+m)\right] (10)$$

and θ_{δ} is vector of parameters

$$\boldsymbol{\theta}_{\delta}^{T}(k) = \begin{bmatrix} a_{0}', a_{1}', ..., a_{n-1}', b_{0}', b_{1}', ..., b_{m}' \end{bmatrix}$$
(11)

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

2.2 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 three different recursive identification methods were used and they are shown beneath.

Ordinary Recursive Least Squares (ORLS) method is one of basic identification methods and it can be formally written by the set of equations (Fikar and Mikleš, 1999):

$$\varepsilon(k) = y(k) - \varphi^{T}(k) \cdot \theta(k-1)$$

$$\gamma(k) = \left[1 + \varphi^{T}(k) \cdot \mathbf{P}(k-1) \cdot \varphi(k)\right]^{-1}$$

$$L(k) = \gamma(k) \cdot \mathbf{P}(k-1) \cdot \varphi(k)$$

$$\mathbf{P}(k) = \mathbf{P}(k-1) - \gamma(k) \cdot \mathbf{P}(k-1) \cdot \varphi(k) \cdot \frac{\varphi^{T}(k) \cdot \mathbf{P}(k-1)}{\varphi(k) \cdot \varphi(k)}$$

$$\hat{\varphi}(k) = \hat{\theta}(k-1) + L(k) \varepsilon(k)$$

(12)

Where ε denotes a prediction error and **P** is a covariance matrix.

RLS Method with Exponential Forgetting is modification of ORLS. 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 \mathbf{P} by the equation

$$\mathbf{P}(k) = \frac{1}{\lambda_1(k-1)} \Big[\mathbf{P}(k-1) - \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k) \cdot \boldsymbol{\varphi}^T(k) \cdot \mathbf{P}(k-1)}{\lambda_1(k-1) + \boldsymbol{\varphi}^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k)} \Big] (13)$$

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 λ_1 is computed from the equation

$$\lambda_{1}(k) = 1 - K \cdot \gamma(k) \cdot \varepsilon^{2}(k) \qquad (14)$$

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

RLS with Directional Forgetting (Kulhavy a Karny, 1984) is used in the cases where RLS methods with exponential forgetting can become unstable. In this case, parameters are being forgotten only in the direction from which new information came. A computation algorithm can be formulated by the following equations:

$$r(k-1) = \boldsymbol{\varphi}^{T}(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k)$$
$$\boldsymbol{L}(k) = \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k)}{1+r(k-1)}$$
$$\beta(k-1) = \begin{cases} \lambda_{1}(k-1) - \frac{1-\lambda_{1}(k-1)}{r(k-1)} \text{ for } r(k-1) > 0 & (15) \\ 1 & \text{ for } r(k-1) = 0 \end{cases}$$
$$\mathbf{P}(k) = \mathbf{P}(k-1) - \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k) \cdot \boldsymbol{\varphi}^{T}(k) \cdot \mathbf{P}(k-1)}{\beta(k-1)^{-1} + r(k-1)}$$

Where λ_1 is computed similar as in Eq. (14).

2.3 Control System Configuration

There were used two control system configurations displayed in Fig. 1 and Fig. 2. The first configuration with one degree-of-freedom (1DOF) shown in Fig. 1 has controller Q only in the feedback segment.



Fig. 1: 1DOF control configuration



Fig. 2: 2DOF control configuration

On the other hand, configuration with two degreesof-freedom (2DOF) in Fig. 2 has one part of the controller in the feedback segment -Q and the second part *R* of the controller is in feedforward segment.

G in both configurations 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.

2.4 Polynomial methods

Transfer functions of the feedback (Q) and feedforward (R) parts of the controller are

$$Q(s) = \frac{q(s)}{s \cdot p(s)}; R(s) = \frac{r(s)}{s \cdot p(s)}$$
(16)

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

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

$$t(s) \cdot s + b(s) \cdot r(s) = d(s)$$
(17)

Parameters of the polynomials a(s) and b(s) are known from the recursive identification and polynomial d(s) is a stable polynomial. Polynomial t(s) in the second diophantine equation is an additive stable polynomial with random coefficients, because these coefficients are not used for computing of coefficients of the polynomial r(s) in 2DOF configuration. All these equations are valid for step changes of the reference and disturbance signals.

The feedback controller Q(s) ensures stability, load disturbance attenuation for both configurations and asymptotic tracking for 1DOF configuration. On the other hand, feedforward part R(s) ensures asymptotic tracking in 2DOF configuration. A demand for a stable controller is fulfilled if the polynomial p(s) in the denominators of (16) is stable. Inner properness holds if all transfer functions are proper. Transfer function Q(s) in (16) is proper if

$$\deg q \le \deg p + 1 \tag{18}$$

Degrees of the polynomials p and q are computed with respect to conditions (2), (18) and solvability of the diophantine equations (17) as follows

$$\deg q = \deg a, \deg p \ge \deg a - 1, \deg r = 0 \quad (19)$$

Roots of the polynomial d(s) on the right side of the equations (17) 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 (17). One approach is to choose *n* different or multiple roots

$$d(s) = (s + \alpha)^{m}; d(s) = (s + \alpha_{1})^{m/2} \cdot (s + \alpha_{2})^{m/2} \dots (20)$$

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

This method has one disadvantage, there is no rule how to choose roots α . 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

$$J = \frac{1}{2\pi j} \int_{-j\omega}^{j\omega} \left\{ E^*(s) \mu_w E(s) + \tilde{U}^*(s) \varphi_w \tilde{U}(s) \right\} ds \quad (21)$$

Where $\varphi_w > 0$ and $\mu_w \ge 0$ 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

$$d(s) = g(s) \cdot n(s) \tag{22}$$

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

$$(a \cdot f)^* \cdot \varphi_w \cdot a \cdot f + b^* \cdot \mu_w \cdot b = g^* \cdot g$$

$$n^* \cdot n = a^* \cdot a$$
(23)

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

$$\deg d = \deg(g \cdot n) = 2\deg a + 1 \tag{24}$$

3 SIMULATION EXPERIMENT

Proposed control strategy was validated by the simulation experiment on the nonlinear system represented by the 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):

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$2A \xrightarrow{k_3} D$$
(25)

The graphical scheme of this reactor can be seen in Fig. 3



Fig. 3: Continuous Stirred Tank Reactor (CSTR)

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

$$\frac{dc_A}{dt} = \frac{q_r}{V_r} (c_{A0} - c_A) - k_1 c_A - k_3 c_A^2 \qquad (26)$$

$$\frac{dc_B}{dt} = -\frac{q_r}{V_r}c_B + k_1c_A - k_2c_B \tag{27}$$

$$\frac{dT_r}{dt} = \frac{q_r}{V_r} (T_{r0} - T_r) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}} (T_c - T_r) (28)$$
$$\frac{dT_c}{V_r} = \frac{1}{(Q_r + A U (T_r - T_r))} (29)$$

 $m_c c_{pc} \bigvee_{c} c_{c}$ dt 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.

Table 1. Parameters of the reactor	
$k_{01} = 2.145 \cdot 10^{10} min^{-1}$	$k_{02} = 2.145 \cdot 10^{10} min^{-1}$
$k_{03} = 1.5072 \cdot 10^8 min^{-1}.mol^{-1}$	$E_1/R = 9758.3 K$
$E_2/R = 9758.3 K$	$E_3/R = 8560 K$
$h_1 = -4200 \ kJ.kmol^{-1}$	$h_2 = 11000 \ kJ.kmol^{-1}$
$h_3 = 41850 \ kJ.kmol^{-1}$	
$V_r = 0.01 \ m^3$	$\rho_r = 934.2 \ kg.m^{-3}$
$c_{pr} = 3.01 \ kJ.kg^{-1}.K^{-1}$	$q_r = 2.365 \cdot 10^{-3} m^3 min^{-1}$
$c_{pc} = 2.0 \ kJ.kg^{-1}.K^{-1}$	$Q_c = -18.5583 \ kJ.min^{-1}$
$U = 67.2 \ kJ.min^{-1}m^{-2}K^{-1}$	$A_r = 0.215 \ m^2$

 $c_{A0} = 5.1 \ kmol.m^{-3}$

 $T_{r0} = 387.05 K$

The reaction heat (h_r) in eq. (28) is expressed as:

 $h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B + h_3 \cdot k_3 \cdot c_A^2$ (30)where h_i means reaction enthalpies.

 $c_{B0} = 0 \ kmol.m^{-3}$

 $m_c = 5 \ kg$

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

$$k_j(T_r) = k_{0j} \cdot \exp\left(\frac{-E_j}{RT_r}\right), \text{ for } j = 1, 2, 3 \quad (31)$$

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

Static analysis has shown (Vojtesek, et al., 2004), that system has an optimal working point for volumetric flow rate of the reactant $q_r = 2.365 \times 10^{-3}$ $m^3.min^{-1}$ a heat removal $Q_c = -18.56 \ kJ.min^{-1}$. 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.

$$y(t) = T_{r}(t) - T_{r}^{s}(t) [K]$$

$$u(t) = 100 \cdot \frac{Q_{c}(t) - Q_{c}^{s}(t)}{Q_{c}^{s}(t)} [\%]$$
(32)

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

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0}$$
(33)

Equation (33) can be rewritten for the identification to the form of the differential equation

$$y_{\delta}(k) = -a_{1}y_{\delta}(k-1) - a_{0}y_{\delta}(k-2) + b_{1}u_{\delta}(k-1) + b_{0}u_{\delta}(k-2)$$
(34)

where y_{δ} is recomputed output to the δ -model: $y_{\delta}(k) = \frac{y(k) - 2y(k-1) + y(k-2)}{m^2}$

$$y_{\delta}(k-1) = \frac{y(k-1) - y(k-2)}{T_{v}} \qquad u_{\delta}(k-1) = \frac{u(k-1) - u(k-2)}{T_{v}}$$
(35)
$$y_{\delta}(k-2) = y(k-2) \qquad u_{\delta}(k-2) = u(k-2)$$

where T_{ν} is the sampling period, the data vector is $\phi^{T}(k-1) = \left[-y_{\delta}(k-1), -y_{\delta}(k-2), u_{\delta}(k-1), u_{\delta}(k-2)\right]$ (36) and the vector of estimated parameters

$$\hat{\Theta}^{T}\left(k\right) = \left[\hat{a}_{1}, \hat{a}_{0}, \hat{b}_{1}, \hat{b}_{0}\right]$$
(37)

could be computed from the ARX (Auto-Regressive eXtrogenous) model

$$y_{\delta}(k) = \hat{\Theta}^{T}(k)\phi(k-1)$$
(38)

by the recursive least squares methods described in part 2.2.

Degrees of the polynomials p(s), q(s) r(s) and d(s) are then computed via (19) and (24):

 $\deg q = 2; \deg p = 2; \deg r = 0; \deg d = 5$ (39)

Polynomials g(s) and n(s) in the equation (22) are

$$g(s) = g_3 s^3 + g_2 s^2 + g_1 s + g_0$$

$$n(s) = s^2 + n_1 s + n_0$$
(40)

and their coefficients are computed as

$$g_{0} = \sqrt{\mu_{w}b_{0}^{2}}, g_{1} = \sqrt{2g_{0}g_{2}} + \varphi_{w}a_{0}^{2} + \mu_{w}b_{1}^{2},$$

$$g_{2} = \sqrt{2g_{1}g_{3}} + \varphi_{w}(a_{1}^{2} - 2a_{0}), g_{3} = \sqrt{\varphi_{w}}, \quad (41)$$

$$n_{0} = \sqrt{a_{0}^{2}}, n_{1} = \sqrt{2n_{0} + a_{1}^{2} - 2a_{0}}$$

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

$$Q(s) = \frac{q_2 s^2 + q_1 s + q_0}{s(s^2 + p_1 s + p_0)}; R(s) = \frac{r_0}{s(s^2 + p_1 s + p_0)} (42)$$

Where parameters of the polynomials q(s) and p(s) by the comparison of the coefficients of the *s*-powers a in diophantine equations (17).

4. SIMULATION RESULTS

All simulation experiments took 500 min and 5 step changes were done during this interval. The first simulation study was done for various values of the weighting factor ϕ_w in (41) for both 1DOF and 2DOF configurations. As you can see in Fig. 4, simulation is quicker with the decreasing value of the factor ϕ_w . On the other hand, a low value of ϕ_w results in small overshoots of the output response. Output responses for 2DOF configuration in Fig. 5 have 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.

Fig. 6 compares control with 1DOF and 2DOF for weighting factor $\phi_w = 0.02$. As it can be seen, the only difference is that 2DOF has better behaviour at the beginning in this case. The second advantage is that 2DOF has a smoother course of the action value – see Fig. 7. On the contrary, 1DOF configuration is a little bit quicker than 2DOF.



Fig. 4: Course of the output variable y(t) for various weighting factors ϕ_w , 1DOF configuration



Fig. 5: Course of the output variable y(t) for various weighting factors ϕ_w , 2DOF configuration



Fig. 6: Course of the output variable y(t) for 1DOF and 2DOF configurations, $\phi_w = 0.02$

The last analysis was done for three recursive least squares methods described in part 2.2. Fig. 8 clearly shows, that usage of forgetting has no effect on the output response which is the same for all identifications. Fig. 9 shows course of the identified parameters during the control which again is the same for all types of identifications. Identification has problems only at the very beginning and that is why the data in Fig. 9 are cut.



Fig. 7: Course of the input variable u(t) for 1DOF and 2DOF configurations, $\phi_w = 0.02$



Fig. 8: Course of the output variable y(t) for various types of identification, $\phi_w = 0.02$



Fig. 9: Course of the identified parameters a'_1 , a'_0 , b'_1 and b'_0 for various of identification, $\phi_w = 0.02$

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 ϕ_w but there should be some small overshoots for low value of ϕ_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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