Simulation of nonlinear adaptive control of a continuous stirred tank reactor

Petr Dostál, Vladimír Bobál, and František Gazdoš

Abstract—The paper presents design and simulation results of nonlinear adaptive control of a chemical reactor. The control strategy appears from factorization of the controller on an adaptive dynamic linear part and a static nonlinear part. The static nonlinear part is derived on the basis of simulated steady-state characteristics of the process and its subsequent inversion and approximation. The linear part consisting of two linear feedback controllers results from an approximation of nonlinear elements in the control system by an external linear model with recursively estimated parameters. The control law is derived via the polynomial approach and the pole placement method.

Keywords—Nonlinear process, steady-state characteristics, external linear model, parameter estimation, polynomial approach.

I. INTRODUCTION

CONTINUOUS stirred tank reactors (CSTRs) are units frequently used in chemical and biochemical industry. From the system theory point of view, CSTRs belong to a class of nonlinear systems with mathematical models described by sets of nonlinear differential equations. Their models are derived and described in e.g. [1], [2] and [3].

It is well known that the control of chemical reactors often represents very complex problem. The control problems are due to the process nonlinearity and high sensitivity of the state and output variables to input changes. In addition, the dynamic characteristics may exhibit a varying sign of the gain in various operating points as well as non-minimum phase behaviour. Even if some processes with weaker nonlinearities are controllable also by conventional controllers, e.g. [4], the most part of nonlinear processes requires application some of advanced methods.

One possible method to cope with this problem exploits linear adaptive controllers with parameters computed and readjusted on the basis of recursively estimated parameters of an appropriate chosen continuous-time external linear model (CT ELM) of the process. Some results obtained by this method can be found in e.g. [5], [6] and [7].

An effective approach to the control of CSTRs and similar processes utilizes various methods of the nonlinear control (NC). Several modifications of the NC theory are described in e.g. [8]–[12]. Especially, a large class of the NC methods exploits linearization of nonlinear plants, e.g. [13], an application of PID controllers, e.g. [14], [15], or factorization of nonlinear models of the plants on linear and nonlinear parts, e.g. [16]–[21].

In this paper, the CSTR control strategy is based on an application of the controller consisting of a static nonlinear part (SNP) and an adaptive dynamic linear part (DLP). The static nonlinear part is obtained from simulated or measured steady-state characteristic of the CSTR, its inversion, exponential approximation, and, subsequently, its differentiation. On behalf of development of the linear part, the SNP including the nonlinear model of the CSTR is approximated by a CT external linear model. For the CT ELM parameter estimation, the direct estimation in terms of filtered variables is used, see e.g. [22] and [23]. The method is based on filtration of continuous-time input and output signals where the filtered variables have in the s-domain the same properties as their non-filtered counterparts.

The DLP structure with two feedback controllers is considered. Such structure was described in e.g. [24] and [25]. Then, the resulting CT controllers are derived using the polynomial approach [26] and the pole placement method.

The simulations are performed on a nonlinear model of the CSTR with a first order consecutive exothermic reaction.

II. MODEL OF THE CSTR

Consider a CSTR with the first order consecutive exothermic reaction according to the scheme A \( \xrightarrow{k_1} \) B \( \xrightarrow{k_2} \) C and with a perfectly mixed cooling jacket. Using usual simplifications, the model of the CSTR is described by four nonlinear differential equations

\[
\frac{dc_A}{dt} = -\left(\frac{q_f}{V_T} + k_1\right)c_A + \frac{q_f}{V_T}c_{Af}
\]

\[
\frac{dc_B}{dt} = -\left(\frac{q_f}{V_T} + k_2\right)c_B + k_1c_A + \frac{q_f}{V_T}c_{Bf}
\]

\[
\frac{dT_r}{dt} = \frac{h}{\rho c_p} + \frac{q_f(T_r - T_j)}{V_T} + \frac{A_k U}{V_T(\rho c_p)}(T_c - T_r)
\]
\[
\frac{dT}{dt} = \frac{q_c}{V_c} (T_{cl} - T_c) + \frac{A_h U}{V_c \rho c_p} (T_r - T_c)
\]

(4)

with initial conditions \( c_A(0) = c^0_A, \ c_B(0) = c^0_B \), \( T_i(0) = T^i_r \) and \( T_c(0) = T^0_c \). Here, \( t \) is the time, \( c \) stands for concentrations, \( T \) for temperatures, \( V \) for volumes, \( \rho \) for densities, \( c_p \) for specific heat capacities, \( q \) for volumetric flow rates, \( A_h \) for the heat exchange surface area and \( U \) for the heat transfer coefficient.

The subscripts denoted \( r \) describe the reactant mixture, \( c \) the coolant, \( f \) the steady-state inputs and the superscript \( s \) the initial conditions. Reaction rates and reaction heat are expressed as

\[
k_j = k_0 j \exp \left( -\frac{E_j}{RT_j} \right), \quad j = 1, 2
\]

(5)

\[
h_i = h_1 k_1 c_A + h_2 k_2 c_B
\]

(6)

where \( k_0 \) are pre-exponential factors, \( E \) activation energies and \( h \) are reaction entalpies. The values of all parameters, inlet values and steady-state values with used units are given in Tab. 1.

**TABLE I**

<table>
<thead>
<tr>
<th>Parameters, Steady-State Inputs and Initial Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_c = 1.2 \text{ m}^3 )</td>
</tr>
<tr>
<td>( V_c = 0.64 \text{ m}^3 )</td>
</tr>
<tr>
<td>( \rho = 985 \text{ kg m}^{-3} )</td>
</tr>
<tr>
<td>( \rho_c = 998 \text{ kg m}^{-3} )</td>
</tr>
<tr>
<td>( k_{cl} = 5.616 \times 10^{14} \text{ min}^{-1} )</td>
</tr>
<tr>
<td>( k_{cl} = 1.128 \times 10^{14} \text{ min}^{-1} )</td>
</tr>
<tr>
<td>( h_1 = 4.8 \times 10^4 \text{ kJ kmol}^{-1} )</td>
</tr>
<tr>
<td>( c_A^0 = 1.5796 \text{ kmol m}^{-3} )</td>
</tr>
<tr>
<td>( T_r^0 = 324.80 \text{ K} )</td>
</tr>
<tr>
<td>( c_{Af} = 2.85 \text{ kmol m}^{-3} )</td>
</tr>
<tr>
<td>( T_{r,c} = 323 \text{ K} )</td>
</tr>
<tr>
<td>( q_{cl} = 0.08 \text{ m}^3 \text{ min}^{-1} )</td>
</tr>
</tbody>
</table>

In term of the practice, only the coolant flow rate can be taken into account as the control input. As the controlled output, the reactant temperature is considered. For the control purposes, the control input \( u(t) \) and the controlled output \( y(t) \) are defined as deviations from steady values

\[
u(t) = q_{cl}(t) - q_{cl}^s, \quad y(t) = T_i(t) - T_c^s
\]

(7)

The dependence of the reactant temperature on the coolant flow rate in the steady-state is in Fig. 1. In subsequent control simulations, the operating interval for \( q_c \) has been determined as

\[
q_{c,\text{min}} \leq q_c(t) \leq q_{c,\text{max}}
\]

(8)

With regard to the purposes of a latter steady-state characteristic approximation, the values \( q_{cl} \) and \( q_{cl,\text{U}} \) are established that denote the lower and upper bound of \( q_c^s \) used for the approximation, and, \( T_{r,\text{U}} \) and \( T_{r,\text{L}} \) to them corresponding temperatures.

III. CONTROLLER DESIGN

As previously introduced, the controller consist of a static nonlinear part and a dynamic linear part as shown in Fig. 2.

![Controller scheme](image)

**Fig. 2** The controller scheme.

The DLP creates a linear dynamic relation between the reference signal \( w(t) \) and \( u_0(t) = \Delta T_{r,w}(t) \) which represents a difference of the reactant temperature adequate to its desired value. Then, the SNP generates a static nonlinear relation between \( u_0 \) and a corresponding increment (decrement) of the coolant flow rate.

**A. Nonlinear part of the controller**

The SNP derivation appears from a simulated or measured steady-state characterististics. The coordinates on the graph axis are defined as

\[
y = \frac{q_{c}^s - q_{cl}}{q_{cl}}, \quad \psi = T_i^s - T_{r,c}
\]

(9)

where \( q_{cl} \) is the lower bound in the interval

\[
q_{cl} \leq q_{c}^s \leq q_{cl,\text{U}}
\]

(10)

and, \( T_{r,c} \) is the temperature corresponding to \( q_{cl,\text{U}} \).

It can be recommended to select the interval (10) slightly longer than (8). In this paper, lower and upper values in (8) and (10) were chosen \( q_{cl} = 0.016, \ q_{cl,\text{min}} = 0.02 \), \( q_{cl,\text{max}} = 0.12 \) and \( q_{cl,\text{U}} = 0.13 \).

In term of the practice, it can be supposed that the measured data will be affected by measurement errors. The simulated steady-state characteristic that corresponds to reality is shown in Fig. 3.

![Operating point](image)

**Fig. 1** Dependence of the reactant temperature on the coolant flow rate in the steady-state.
Changing the axis, the inverse of this characteristic can be approximated by a function from the ring of polynomial, exponential, rational, eventually, by other type functions. Here, the second order exponential approximate function has been found in the form

\[ \gamma = -74071.7 + 2.4589 \exp\left(\frac{-\psi}{3.967}\right) + 74076 \exp\left(\frac{-\psi}{697475}\right) \]  

The inverse characteristic together with its approximation is in Fig. 4.

A difference of the coolant flow rate \( u(t) = \Delta q_c(t) \) in the output of the SNP can be computed for each \( T_r \) as

\[ u(t) = \Delta q_c(t) = q_{cl} \left( \frac{d\gamma}{d\psi}\right)_{\psi(T_r)} u_0(t) \]  

The derivative of the approximate function (11) takes the form

\[ \frac{d\gamma}{d\psi} = -0.6198 \exp\left(\frac{-\psi}{3.967}\right) - 0.1062 \exp\left(\frac{-\psi}{697475}\right) \]  

Its plot is in Fig. 5.

B. CT external linear model of nonlinear elements

A structure of the CT ELM of the SNP in conjunction with a nonlinear model of the CSTR was chosen on the basis of step responses simulated in a neighborhood of the operating point \( (q_c^0 = 0.08 \text{ m}^3\text{min}^{-1}, T_r^0 = 324.8 \text{ K}) \). The step responses for some step changes of \( u_0 \) are shown in Fig. 6.

For all responses, the gain of the SNP+CSTR system has been computed as \( g_s = \lim_{t \to \infty} \frac{y(t)}{u_0} \).

Taking into account profiles of curves in Fig. 6 with zero derivatives in \( t = 0 \), the second order CT ELM has been chosen in the form of the second order linear differential equation

\[ \dot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_0 u_0(t) \]  

or, in the transfer function representation as

\[ G(s) = \frac{Y(s)}{U(s)} = \frac{b(s)}{a(s) s^2 + a_1 s + a_0} \]  

where \( s \) is the complex variable (parameter of the Laplace transform).

C. CT ELM parameter estimation

The method of the CT ELM parameter estimation can be briefly carried out as follows.

Since the derivatives of both input and output cannot be directly measured, filtered variables \( u_{0f} \) and \( y_f \) are established as the outputs of filters

\[ c(\sigma) u_{0f}(t) = u_0(t) \]
\( c(\sigma) y(t) = y(t) \quad (16) \)

where \( \sigma = d/dt \) is the derivative operator, \( c(\sigma) \) is a stable polynomial in \( \sigma \) that fulfills the condition \( \text{deg} \ c(\sigma) \geq \text{deg} \ a(\sigma) \). It can be easily proved that the transfer behavior among filtered and among nonfiltered variables are equivalent. Using the \( L \)-transform of (15) and (16), the expressions

\[
\begin{align*}
c(s)U_0(s) &= U_0(s) + \mu_t(s) \\
c(s)Y(s) &= Y(s) + \mu_t(s)
\end{align*}
\]

(17) and (18)

\( c(s)Y_t(s) = Y(s) + \mu_t(s) \)

(18)

can be obtained with \( \mu_t \) and \( \mu_e \) as polynomials of initial conditions. Substituting (17) and (18) into (14), and, after some manipulations, the relation between transforms of the filtered input and output takes the form

\[
Y_t(s) = \frac{b(s)}{a(s)} U_0(s) + M(s) = G(s) U_0(s) + M(s)
\]

(19)

where \( M(s) \) is a rational function as the transform of any function \( \mu(t) \) which expresses an influence of initial conditions of filtered variables.

The filtered variables including their derivatives can be sampled from filters (15) and (16) in discrete time intervals \( t = k T_s \), \( k = 0, 1, 2, \ldots \) where \( T_s \) is the sampling period. Denoting \( \text{deg} \ a = n \) and \( \text{deg} \ b = m \), the regression vector is defined as

\[
\Phi(t_k) = \begin{bmatrix} -y_t^{(1)}(t_k) & \ldots & -y_t^{(n-1)}(t_k) \\ u_{0t}(t_k) & \ldots & u_{0t}^{(m)}(t_k) \end{bmatrix}
\]

(20)

Now, the vector of parameters

\[
\Theta^T(t_k) = \begin{bmatrix} a_0 & a_1 & \ldots & a_{n-1} & b_0 & b_1 & \ldots & b_m \end{bmatrix}
\]

(21)

can be estimated from the ARX model

\[
y_t^{(n)}(t_k) = \Theta^T(t_k) \Phi(t_k) + \mu(t_k)
\]

(22)

D. Linear part of the controller

The DLP is inserted into the control loop as shown in Fig. 7. In the scheme, \( w \) is the reference signal, \( v \) is the disturbance, \( y \) is the controlled output, \( u_0 \) is the input to the CT ELM and \( e \) is the tracking error.

The transfer function \( G(s) \) of the ELM is given by (14).

The controller design described in this section appears from the polynomial approach. General conditions required to govern the control system properties are formulated as strong stability (in addition to the control system stability, also the stability of controllers is required), internal properness, asymptotic tracking of the reference and load disturbance attenuation.

The procedure to obtain admissible controllers can be briefly described as follows:

Establish the polynomial \( t \) as

\[
t(s) = r(s) + \tilde{q}(s).
\]

(23)

Then, the control system stability is ensured when polynomials \( \tilde{p} \) and \( t \) are given by a solution of the polynomial equation

\[
a(s) \tilde{p}(s) + b(s) t(s) = d(s)
\]

(24)

with a stable polynomial \( d \) on the right side. Evidently, the roots of \( d \) determine poles of the closed-loop.

Further, the asymptotic tracking and load disturbance attenuation are provided by polynomials \( \tilde{p} \) and \( \tilde{q} \) having the form

\[
\tilde{p}(s) = s p(s), \quad \tilde{q}(s) = s q(s).
\]

(25)

Subsequently, the transfer functions of controllers take forms

\[
Q(s) = \frac{q(s)}{p(s)}, \quad R(s) = \frac{r(s)}{s p(s)}.
\]

(26)

A stable polynomial \( p(s) \) in denominators of (26) ensures the stability of controllers.

The control system satisfies the condition of internal properness when the transfer functions of all its components are proper. Consequently, the degrees of polynomials \( q \) and \( r \) must fulfill inequalities

\[
\text{deg} q \leq \text{deg} p, \quad \text{deg} r \leq \text{deg} p + 1.
\]

(27)

Now, the polynomial \( t \) can be rewritten into the form

\[
t(s) = r(s) + s q(s).
\]

(28)

Taking into account solvability of (24) and conditions (27), the degrees of all unknown polynomials can be easily derived as

\[
\text{deg} t = \text{deg} r = \text{deg} a, \quad \text{deg} q = \text{deg} a - 1,
\]

\[
\text{deg} p \geq \text{deg} a - 1, \quad \text{deg} d \geq 2 \text{deg} a.
\]

(29)

Denoting \( \text{deg} \ a = n \), polynomials \( t, r \) and \( q \) have forms

\[
t(s) = \sum_{i=0}^{n} t_i s^i, \quad r(s) = \sum_{i=0}^{n} r_i s^i, \quad q(s) = \sum_{i=1}^{n} q_i s^{i-1}
\]

(30)

where their coefficients fulfill equalities

\[
r_0 = t_0, \quad r_i + q_i = t_i \quad \text{for} \quad i = 1, \ldots, n.
\]

(31)

Then, unknown coefficients \( r_i \) and \( q_i \) can be obtained by a
choice of selectable coefficients \( \beta_i \in \{0,1\} \) such that
\[
q_i = \beta_i t_i, \quad q_i = (1 - \beta_i) t_i \quad \text{for} \quad i = 1, \ldots, n.
\] (32)

The coefficients \( \beta_i \) split a weight between numerators of transfer functions \( Q \) and \( R \). With respect to (26) and (32), it may be expected that higher values of \( \beta_i \) will speed up control responses to step references.

**Remark:** If \( \beta_i = 1 \) for all \( i \), the control system in Fig. 1 simplifies to the 1DOF control configuration. If \( \beta_i = 0 \) for all \( i \) and both reference and load disturbance are step functions, the control system corresponds to the 2DOF control configuration.

The controller parameters then follow from solution of the polynomial equation (24) and depend upon coefficients of the polynomial \( d \).

For the second order model (14) with \( \deg a = 2 \), the controller transfer functions (26) take forms
\[
Q(s) = \frac{q_2 s + q_1}{s + p_0}, \quad R(s) = \frac{r_2 s + r_1 + r_0}{s(s + p_0)}.
\] (33)

A required control quality can be achieved by a suitable determination of the polynomial \( d \) on the right side of (24). In this paper, the polynomial \( d \) with roots determining the closed-loop poles is chosen as a product of two stable factors
\[
d(s) = n(s)(s + \alpha)^2
\] (34)

where the polynomial \( n \) is the second order stable polynomial
\[
n(s) = s^2 + n_1 s + n_0
\] (35)
resulting from spectral factorization
\[
a^+(s) a(s) = n^+(s) n(s)
\] (36)
and with coefficients
\[
n_0 = \sqrt{a_0^2}, \quad n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0}.
\] (37)

The selectable parameter \( \alpha \) in (34) can usually be chosen in way of simulation experiments. Note that a choice of \( d \) in the form (34) provides the control of a good quality for aperiodic controlled processes.

The controller parameters can be obtained from a solution of the polynomial equation (24). After some manipulations and using the uncertain coefficient method, the parameters \( p_0 \) and \( t \) are given by the matrix equation
\[
\begin{pmatrix} 1 & 0 & 0 & 0 \\ a_1 & b_0 & 0 & 0 \\ a_0 & 0 & b_0 & 0 \\ 0 & 0 & 0 & b_0 \end{pmatrix} \begin{pmatrix} p_0 \\ t_2 \\ t_1 \\ t_0 \end{pmatrix} = \begin{pmatrix} d_3 - a_1 \\ d_2 - a_0 \\ d_1 \\ d_0 \end{pmatrix}
\] (38)

where
\[
d_3 = n_1 + 2\alpha, \quad d_2 = 2\alpha n_1 + n_0 + \alpha^2
\]
\[
d_1 = 2\alpha n_0 + \alpha^2 n_1, \quad d_0 = \alpha^2 n_0
\] (39)

The controller parameters in (33) can then be computed as
\[
r_1 = \beta_1 t_1, \quad r_2 = \beta_2 t_2, \quad q_1 = (1 - \beta_1) t_1, \quad q_2 = (1 - \beta_2) t_2.
\] (40)

Now, it follows from the above introduced procedure that the parameters of both controllers depend upon coefficients \( \beta \) affecting the numerators in (33) as well as upon the parameter \( \alpha \) which affects the closed-loop poles. Consequently, tuning of the controllers can be performed by a suitable choice of the selectable parameters \( \beta \) and \( \alpha \).

The complete adaptive control system is is shown in Fig. 8.

![Fig. 8 Adaptive control system.](image)

**IV. CONTROL SIMULATIONS**

The control simulations were performed in the vicinity of the operating point (\( q_c = 0.08 \text{ m}^3\text{min}^{-1}, \quad T_{c} = 324.8 \text{ K} \)). For the start (the adaptation phase), a P controller with a small gain was used in all simulations.

The simulated control responses for different values \( \beta \) including their limiting values (\( \beta_1 = \beta_2 = 0, \quad \beta_1 = \beta_2 = 1 \)) are shown in Figs. 9 – 13. The effect of parameters \( \beta \) is evident. Their increase speeds up the control, but, it can lead to overshoots of the controlled output. Moreover, their greater values cause higher control inputs and their changes. This fact is important for a practical control where greater input changes may be undesirable.

The effect of the pole \( \alpha \) on the control responses is transparent from Figs. 14–16. Here, on the basis of precomputed simulations, two values of \( \alpha \) were selected. The control results show sensitivity of the controlled output and the input signals to \( \alpha \). Obviously, careless selection of this parameter can lead to controlled outputs with overshoots and oscillations (here for \( \alpha > 0.2 \)). Moreover, an increasing \( \alpha \) leads to higher values and changes of the input signals. This fact can be important in control of some reactors where expressive input changes are undesirable.

Evolution of the DLP parameters during control is shown in Fig. 17.
Fig. 9 Controlled outputs in 1DOF and 2DOF control structures ($\alpha = 0.15$).

Fig. 10 Coolant flow rates in 1DOF and 2DOF control structures ($\alpha = 0.15$).

Fig. 11 Controlled outputs for various $\beta_1$ ($\beta_2 = 0, \alpha = 0.1$).

Fig. 12 Outputs from DLP for various $\beta_1$ ($\beta_2 = 0, \alpha = 0.1$).

Fig. 13 Coolant flow rates during control for various $\beta_1$ ($\beta_2 = 0, \alpha = 0.1$).

Fig. 14 Controlled outputs for various $\alpha$ ($\beta_2 = 0, \beta_1 = 1$).

Fig. 15 Outputs from DLP for various $\alpha$ ($\beta_2 = 0, \beta_1 = 1$).

Fig. 16 Coolant flow rates during control for various $\alpha$ ($\beta_2 = 0, \beta_1 = 1$).
A presence of the integrating part in the DLP enables rejection of various step disturbances entering into the process. Here, step disturbances \( \Delta c_{A_f} = \pm 0.1 \text{kmol m}^{-3} \) at times \( t_{c1} = 250 \text{min} \) and \( t_{c2} = 650 \text{min} \) were injected into the CSTR. The DLP parameters were estimated only in the first (tracking) interval \( t < 200 \text{min} \). The experiences of authors of this paper proved that an utilization of recursive identification in the phase of a constant reference and in a presence of step disturbances decreases the control quality. From this reason, during the interval \( t \geq 200 \text{min} \), fixed DLP parameters were used. The controlled output responses are shown in Fig. 18.

The control simulation results in presence of the additive unmeasured random disturbance \( v(t) = T_{rt} - T_{rA}^{*} \) is shown in Fig. 19. The control responses document an usability of the method also in this case.

An affect of presence of the SNP in the control loop is evident from the control responses shown in Fig. 20. Here, the standard adaptive control without the SNP was compared with the nonlinear adaptive control. Both simulations have been performed under the same conditions for \( \alpha = 0.075 \). The responses show priority of the nonlinear control especially for greater changes of the reference signal.

V. CONCLUSIONS

In this paper, one approach to the nonlinear continuous-time adaptive control of the reactant temperature in a continuous stirred tank reactor was proposed. The control strategy is based on factorization of a controller into the adaptive dynamic linear part and the static nonlinear part. A design of the controller nonlinear part employs simulated or measured steady-state characteristics of the process and their additional modifications. Then, the system consisting of the controller nonlinear part and a nonlinear model of the CSTR is approximated by a continuous time external linear model with parameters obtained through direct recursive parameter estimation. The dynamic linear controller part consists of two continuous time feedback subcontrollers. These ones are derived using the polynomial approach and given by a solution of the polynomial equation. Tuning of its parameters is possible by two types of selectable parameters. The presented method has been tested by computer simulations on the nonlinear model of the CSTR with a consecutive exothermic reaction. Simulation results demonstrated an applicability of
the presented control strategy and its usefulness especially for
greater changes of input signals in strongly nonlinear regions.
It can be expected that the described control strategy is also
suitable for other similar nonlinear technological processes.

REFERENCES