2DOF adaptive control of a tubular chemical reactor

Petr Dostál, Jiří Vojtěšek, Vladimír Bobál, and Zdeněk Babík

Abstract—The paper deals with adaptive control of a tubular chemical reactor. A nonlinear model of the process is approximated by a continuous-time external linear model with parameters estimated using a corresponding delta model. The 2DOF control system structure is considered. The controller design is based on the polynomial approach. The adaptive control is tested on the nonlinear model of the tubular chemical reactor with a consecutive exothermic reaction.

***Keywords*—**Tubular chemical reactor, external linear model, delta model, parameter estimation, polynomial method.

I. Introduction

TUBULAR chemical reactor are units frequently used in chemical industry. From the system theory point of view, tubular chemical reactors belong to a class of nonlinear distributed parameter systems with mathematical models described by sets of nonlinear partial differential equations (NPDRs). The methods of modelling and simulation of such processes are described e.g. in [1] – [5].

It is well known that the control of chemical reactors, and, tubular reactors especially, often represents very complex problem. The control problems are due to the process nonlinearity, its distributed nature, and high sensitivity of the state and output variables to input changes. Evidently, the process with such properties is hardly controllable by conventional control methods, and, its effective control requires application some of advanced methods. Here, various efficient methods may be used as the predictive control, e.g. [6], [7], [8], the robust control, e.g. [9], or nonlinear control, e.g. [10], [11], [12] can be applied.

One possible method to cope with this problem is using adaptive strategies based on an appropriate choice of an continuous-time external linear model (CT ELM) with recursively estimated parameters. These parameters are consequently used for parallel updating of controller's parameters. Some results obtained in this field were presented by authors of this paper in

For the CT ELM parameters estimation, either the direct method [13] or application of an external delta model with the same structure as the CT model can be used. The basics of delta models have been described in e.g. [14], [15]. Although delta models belong into discrete models, they do not have such disadvantageous properties connected with shortening of a sampling period as discrete z-models. In addition, parameters of delta models can directly be estimated from sampled signals. Moreover, it can be easily proved that these parameters converge to parameters of CT models for a sufficiently small sampling period (compared to the dynamics of the controlled process), as shown in [16].

This paper deals with continuous-time adaptive control of a tubular chemical reactor with a countercurrent cooling as a nonlinear single input – single output process. With respect to practical possibilities of a measurement and control, the mean reactant temperature and the coolant flow rate are chosen as the controlled output and the control input. The parameters of its CT ELM are estimated via corresponding delta model. The two degrees of freedom (2DOF) structure of the control system is considered. The resulting controllers are derived using the polynomial approach [17] and the pole assignment method (see, e.g. [18]). The approach is tested on a mathematical model of the tubular chemical reactor.

II. Model of the Reactor

An ideal plug-flow tubular chemical reactor with a simple exothermic consecutive reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ in the liquid phase and with the countercurrent cooling is considered. Heat losses and heat conduction along the metal walls of tubes are assumed to be negligible, but dynamics of the metal walls of tubes are significant. All densities, heat capacities, and heat transfer coefficients are assumed to be constant. Under above assumptions, the reactor model can be described by five PDRs in the form

$$\frac{\partial c_A}{\partial t} + v_r \frac{\partial c_A}{\partial z} = -k_1 c_A \tag{1}$$

$$\frac{\partial c_B}{\partial t} + v_r \frac{\partial c_B}{\partial z} = k_1 c_A - k_2 c_B \tag{2}$$

$$\frac{\partial T_r}{\partial t} + v_r \frac{\partial T_r}{\partial z} = \frac{Q_r}{(\rho c_p)_r} - \frac{4U_1}{d_1(\rho c_p)_r}(T_r - T_w) \tag{3}$$

$$\frac{\partial T_w}{\partial t} = \frac{4}{(d_2^2 - d_1^2)(\rho c_p)_w}\left[d_1 U_1 (T_r - T_w) + \right. \\ \left. + d_2 U_2 (T_c - T_w) \right] \tag{4}$$

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$$\frac{\partial T_c}{\partial t} - v_c \frac{\partial T_c}{\partial z} = \frac{4 n_1 d_2 U_2}{(d_3^2 - n_1 d_2^2)(\rho c_p)_c}(T_w - T_c) \tag{5}$$

with initial conditions

$c_A(z,0) = c_A^s(z)$, $c_B(z,0) = c_B^s(z)$, $T_r(z,0) = T_r^s(z)$,

$T_w(z,0) = T_w^s(z)$, $T_c(z,0) = T_c^s(z)$

and boundary conditions

$c_A(0,t) = c_{A0}(t)$ (kmol/m^3), $c_B(0,t) = c_{B0}(t)$ (kmol/m^3),

$T_r(0,t) = T_{r0}(t)$ (K), $T_c(L,t) = T_{cL}(t)$ (K).

Here, t is the time, z is the axial space variable, c are concentrations, T are temperatures, v are fluid velocities, d are diameters, ρ are densities, c_p are specific heat capacities, U are heat transfer coefficients, n_1 is the number of tubes and L is the length of tubes. The subscript $(\cdot)_r$ stands for the reactant mixture, $(\cdot)_w$ for the metal walls of tubes, $(\cdot)_c$ for the coolant, and the superscript $(\cdot)^s$ for for steady-state values.

The reaction rates and heat of reactions are nonlinear functions expressed as

$$k_j = k_{j0} \exp\left(\frac{-E_j}{R T_r}\right), \quad j = 1, 2 \tag{6}$$

$$Q_r = (-\Delta H_{r1}) k_1 c_A + (-\Delta H_{r2}) k_2 c_B \tag{7}$$

where k_0 are pre-exponential factors, E are activation energies, (- ΔH_r) are in the negative considered reaction entalpies, and R is the gas constant.

The fluid velocities are calculated via the reactant and coolant flow rates as

$$v_r = \frac{4 q_r}{\pi n_1 d_1^2} \ , \ v_c = \frac{4 q_c}{\pi (d_3^2 - n_1 d_2^2)} \tag{8}$$

The parameter values with correspondent units used for simulations are given in Table 1.

TABLE I
USED PARAMETER VALUES

L = 8 m	n_1 = 1200
d_1 = 0.02 m	d_2 = 0.024 m
d_3 = 1 m	
ρ_r = 985 kg/m^3	c_{pr} = 4.05 kJ/kg K
ρ_w = 7800 kg/m^3	c_{pw} = 0.71 kJ/kg K
ρ_c = 998 kg/m^3	c_{pc} = 4.18 kJ/kg K
U_1 = 2.8 kJ/m^{2}s K	U_2 = 2.56 kJ/m^{2}s K
k_{10} = 5.61·10^{16} 1/s	k_{20} = 1.128·10^{18} 1/s
E_1/R = 13477 K	E_2/R = 15290 K
(-ΔH_{r1}) = 5.8·10^4 kJ/kmol	(-ΔH_{r2}) = 1.8·10^4 kJ/kmol

From the system engineering point of view, $c_A(L,t) = c_{A\text{out}}$, $c_B(L,t) = c_{B\text{out}}$, $T_r(L,t) = T_{r\text{out}}$ and $T_c(0,t) = T_{c\text{out}}$ are the output variables, and, $q_r(t)$, $q_c(t)$, $c_{A0}(t)$, $T_{r0}(t)$ and $T_{cL}(t)$ are the input variables. Among them, for the control purposes, mostly the coolant flow rate can be taken into account as the control variable, whereas other inputs enter into the process can be accepted as disturbances. In this paper, the mean reactant temperature given by

$$T_m(t) = \frac{1}{L}\int_0^L T_r(z,t)\,dz \tag{9}$$

is considered as the controlled output.

III. COMPUTATION MODEL

For computation of both steady-state and dynamic characteristics, the finite diferences method is employed. The procedure is based on substitution of the space interval $z \in <0, L>$ by a set of discrete node points $\{z_i\}$ for i = 1, … , n ,and, subsequently, by approximation of derivatives with respect to the space variable in each node point by finite differences. Then, nonlinear PDEs (1) – (5) are approximated by a set of nonlinear ODEs in the form

$$\frac{d c_A(i)}{dt} = -\left[b_0 + k_1(i)\right] c_A(i) + b_0\, c_A(i-1) \tag{10}$$

$$\frac{d c_B(i)}{dt} = k_1(i)\, c_A(i) - \left[b_0 + k_2(i)\right] c_B(i) + \\ + b_0\, c_B(i-1) \tag{11}$$

$$\frac{d T_r(i)}{dt} = b_1 Q_r(i) - (b_0 + b_2) T_r(i) + b_0 T_r(i-1) + \\ + b_2 T_w(i) \tag{12}$$

$$\frac{d T_w(i)}{dt} = b_3\left[T_r(i) - T_w(i)\right] + b_4\left[T_c(i) - T_w(i)\right] \tag{13}$$

$$\frac{d T_c(m)}{dt} = -(b_5 + b_6) T_c(m) + b_5 T_c(m+1) + \\ + b_6 T_w(m) \tag{14}$$

for $i = 1, \ldots, n$ and $m = n - i + 1$, and, with initial conditions

$c_A(i,0) = c_A^s(i)$, $c_B(i,0) = c_B^s(i)$, $T_r(i,0) = T_r^s(i)$, $T_w(i,0) = T_w^s(i)$ and $T_c(i,0) = T_c^s(i)$ for $i = 1, \ldots, n$.

The boundary conditions enter into Eqs. (10) – (14) for i = 1 .Now, nonlinear functions in Eqs. (10) – (14) take the discrete form

$$k_j(i) = k_{j0} \exp\left(\frac{-E_j}{R T_r(i)}\right), \ j = 1, 2 \tag{15}$$

$$Q_r(i) = (-\Delta H_{r1}) k_1(i) c_A(i) + (-\Delta H_{r2}) k_2(i) c_B(i) \tag{16}$$

for i = 1, … , n.

The parameters b in (10) – (14) are calculated from formulas

$$b_0 = \frac{v_r}{h}, \ b_1 = \frac{1}{(\rho c_p)_r}, \ b_2 = \frac{4U_1}{d_1(\rho c_p)_r}, \\ b_3 = \frac{4 d_1 U_1}{(d_2^2 - d_1^2)(\rho c_p)_w}, \ b_4 = \frac{4 d_2 U_2}{(d_2^2 - d_1^2)(\rho c_p)_w}, \\ b_5 = \frac{v_c}{h}, \ b_6 = \frac{4 n_1 d_2 U_2}{(d_3^2 - n_1 d_2^2)(\rho c_p)_c} \tag{17}$$

and, the expression for computation of T_m (9) is rewriten to the discrete form

$$T_m(t) = \frac{1}{n}\sum_{i=1}^{n} T_r(z_i, t) \tag{18}$$

A steady-state model can simply be derived equating the time derivatives in (10) – (14) to zero. Then, after some algebraic modifications, the steady-state model takes the form of difference equations. Computation of the steady-state characteristics is necessary not only for a steady-state analysis but the steady state values $(\cdot)^s(i)$ also constitute initial conditions in ODRs (10) – (14) (here, $(\cdot)$ presents some of variables in the set (10) – (14)).

IV. Steady-state and Dynamic Characteristics

Typical reactant temperature profiles along the reactor tubes computed for $c_{A0}^s = 2.85$, $c_{B0}^s = 0$, $T_{r0}^s = 323$, $T_{c0}^s = 293$ and $q_r^s = 0.15$ for various values of the coolant flow rates are shown in Fig. 1. A presence of a maximum on the reactant temperature profiles is a common property of many tubular reactors with exothermic reactions.

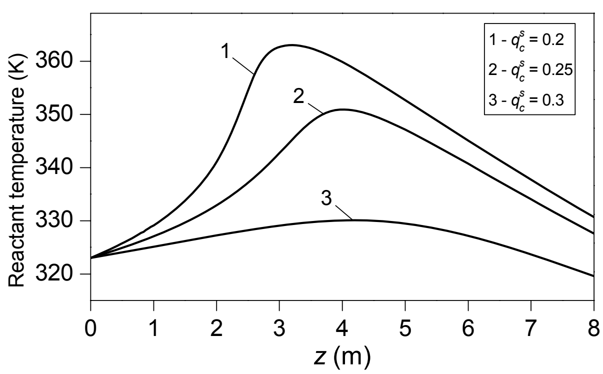

Fig. 1. Reactant temperature profiles for various coolant flow rates.

A dependence of the reactant mean temperature on the coolant flow rate is shown in Fig. 2. The form of the curve documents a nonlinear relation between the reactant mean temperature and the coolant flow rate which will be considered as the controlled output and the control input.

Dynamic charakteristics were computed in the neighbourhood of the chosen operating point $q_c^s = 0.27\ \mathrm{m^3/s}$ and $T_m^s = 334.44\,\mathrm{K}$. The input and the output were considered as deviations from their steady values. Such form is frequently used in the control. The deviations are denoted as follows: $\Delta q_c = q_c(t) - q_c^s$, $\Delta T_m(t) = T_m(t) - T_m^s$.

The responses of the reactant mean temperature to the coolant flow rate step changes are shown in Fig. 3.

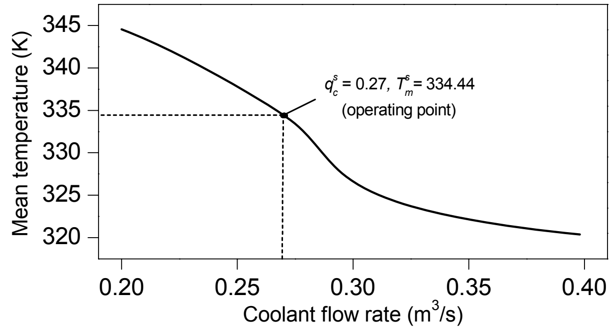

Fig. 2. Dependence of the reactant mean temperature on the coolant flow rates.

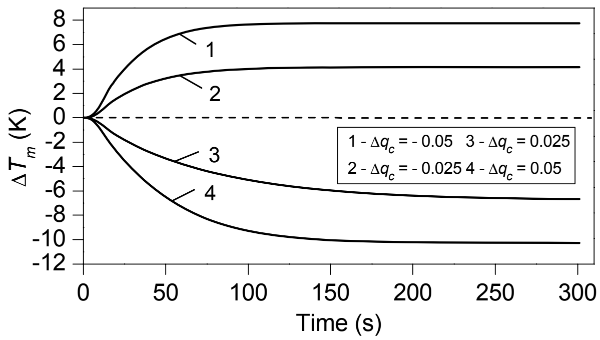

Fig. 3. Reactant mean temperature step responses.

V. CT and Delta External Linear Model

For the control purposes, the controlled output and the control input are defined as

$$y(t) = \Delta T_m(t) = T_m(t) - T_m^s,\ \ u(t) = 10\ \frac{q_c(t) - q_c^s}{q_c^s}. \tag{19}$$

These expressions enable to obtain variables of approximately the same magnitude.

A choice of the CT ELM structure does not stem from known structure of the model (1) – (5) but from a character of simulated step responses. It well known that in adaptive control a controlled process of a higher order can be approximated by a linear model of a lower order with variable parameters. Taking into account profiles of curves in Fig. 3 with zero derivatives in t = 0, the second order CT ELM has been chosen in the form of the second order linear differential equation

$$\ddot{y}(t) + a_1\,\dot{y}(t) + a_0\,y(t) = b_0\,u(t) \tag{20}$$

or, in the transfer function representation as

$$G(s) = \frac{b_0}{s^2 + a_1 s + a_0}. \tag{21}$$

Establishing the δ operator

$$\delta = \frac{q-1}{T_0} \tag{22}$$

where q is the forward shift operator and T_0 is the sampling period, the delta ELM corresponding to (20) takes the form

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$$\delta^2 y(t') + a_1' \delta y(t') + a_0' y(t') = b_0' u(t') \tag{23}$$

where t' is the discrete time.

When the sampling period is shortened, the delta operator approaches the derivative operator, and, the estimated parameters a', b' reach the parameters *a*, *b* of the CT model (20) as shown in [16].

VI. Delta Model Parameter Estimation

Substituting $t' = k-2$, equation (20) may be rewriten to the form

$$\delta^2 y(k-2) + a_1' \delta y(k-2) + a_0' y(k-2) = b_0' u(k-2) \tag{24}$$

In the paper, the recursive identification method with exponential and directional forgetting according to [13] was used.

Establishing the regression vector

$$\mathbf{\Phi}_\delta^T(k-1) = \begin{pmatrix} -\delta y(k-2) & -y(k-2) & u(k-2) \end{pmatrix} \tag{25}$$

where $\delta y(k-2) = \dfrac{y(k-1) - y(k-2)}{T_0}$,

the vector of delta model parameters

$$\mathbf{\Theta}_\delta^T(k) = \begin{pmatrix} a_1' & a_0' & b_0' \end{pmatrix} \tag{26}$$

is recursively estimated from the equation

$$\delta^2 y(k-2) = \mathbf{\Theta}_\delta^T(k) \mathbf{\Phi}_\delta(k-1) + \varepsilon(k) \tag{27}$$

where $\delta^2 y(k-2) = \dfrac{y(k) - 2y(k-1) + y(k-2)}{T_0^2}$.

VII. Controller Design

The 2DOF control system is depicted in Fig. 4.

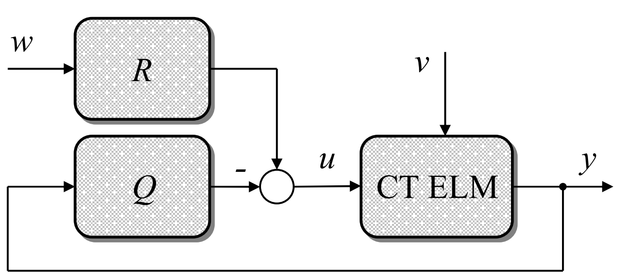

Fig. 4. 2DOF control system.

In the scheme, *w* is the reference signal, *v* denotes the load disturbance, *e* the tracking error, *u* the control input and *y* the controlled output.

The reference *w* and the disturbance *v* are considered as step functions with transforms

$$W(s) = \frac{w_0}{s}, \quad V(s) = \frac{v_0}{s} \tag{28}$$

The transfer functions of both controller parts are in forms

$$R(s) = \frac{r(s)}{p(s)}, \quad Q(s) = \frac{q(s)}{p(s)} \tag{29}$$

where *q*, *r* and *p* are coprime polynomials in s fulfilling the condition of properness $\deg r \le \deg p$ and $\deg q \le \deg p$. For a step disturbance with the transform (28), the polynomial *p* takes the form $p(s) = s\tilde{p}(s)$.

The controller design described in this section follows from the polynomial approach. The general conditions required to govern the control system properties are formulated as follows:

Stability of the control system, internal properness of the control system, asymptotic tracking of the reference and disturbance attenuation.

It is well known that the admissible controller results from the solution of the couple of polynomial equations

$$a(s) s \tilde{p}(s) + b(s) q(s) = d(s) \tag{30}$$

$$t(s) s + b(s) r(s) = d(s) \tag{31}$$

with a stable polynomial *d* on their right sides. The polynomial *t*(*s*) is an auxiliary polynomial which does not enter into the controller design but it is necessary for calculation of (26).

For the transfer function (21) with deg *a* = 2, the degrees of controller polynomials can be derived as

$$\deg q = 2, \deg \tilde{p} = 1, \deg r = 0, \deg d = 4 \tag{32}$$

and, the controller transfer functions take forms

$$Q(s) = \frac{q(s)}{s\tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s(s + p_0)}, \quad R(s) = \frac{r(s)}{s\tilde{p}(s)} = \frac{r_0}{s(s + p_0)}. \tag{33}$$

Moreover, the equality $r_0 = q_0$ can easily be obtained.

The controller parameters then follow from solutions of polynomial equations (30) and (31) and depend upon coefficients of the polynomial *d*.

In this paper, the polynomial *d* with roots determining the closed-loop poles is chosen as

$$d(s) = n(s)(s + \alpha)^2 \tag{34}$$

where *n* is a stable polynomial obtained by spectral factorization

$$a^*(s) a(s) = n^*(s) n(s) \tag{35}$$

and α is the selectable parameter.

Note that a choice of *d* in the form (34) provides the control of a good quality for aperiodic controlled processes.

The coefficients of *n* then are expressed as

$$n_0 = \sqrt{a_0^2}, \quad n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0} \tag{36}$$

and, the controller parameters can be obtained from solution of the matrix equation

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ a_1 & b_0 & 0 & 0 \\ a_0 & 0 & b_0 & 0 \\ 0 & 0 & 0 & b_0 \end{pmatrix} \cdot \begin{pmatrix} p_0 \\ q_2 \\ q_1 \\ q_0 \end{pmatrix} = \begin{pmatrix} d_3 - a_1 \\ d_2 - a_0 \\ d_1 \\ d_0 \end{pmatrix} \tag{37}$$

where

$$\begin{aligned} d_3 &= n_1 + 2\alpha, \; d_2 = 2\alpha n_1 + n_0 + \alpha^2 \\ d_1 &= 2\alpha n_0 + \alpha^2 n_1, \; d_0 = \alpha^2 n_0 \end{aligned} \tag{38}$$

Evidently, the controller parameters can be adjusted by selectable parameter α.

The adaptive control system is shown in Fig. 5.

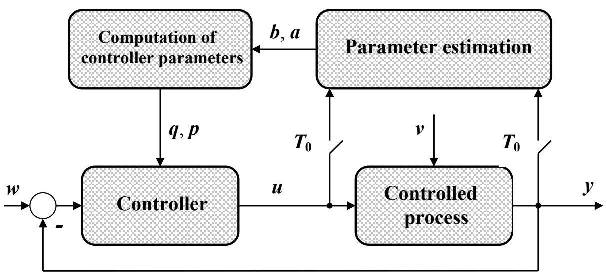

Fig. 5. Adaptive control scheme.

VIII. Control Simulation

Also the control simulations were performed in a neighbourhood of the operating point $q_c^s = 0.27\ \mathrm{m^3/s}$ and $T_m^s = 334.44\,\mathrm{K}$. For the start (the adaptation phase), a P controller with a small gain was used in all simulations.

The effect of the pole α on the control responses is transparent from Figs. 6 and 7. Here, two values of α were selected. The control simulation shows sensitivity of the controlled output and control input to α. There, a difference between controlled output responses is insignificant. However, the control inputs show greater differences in the first time interval. Generally, careless selection of parameter α can lead to controlled output responses of a poor quality or even to the control instability. Moreover, an increasing α leads to higher values and changes of the control input.

As an influence illustration of a additive random disturbance on the control, the control simulated in a presence of the random signal $v(t) = c_{A0}(t) - c_A^s$ is shown in Fig. 8. The simulation result document an usability of the method also in this case.

A presence of the integrating part in the controller enables rejection of various step disturbances entering into the process. Here, step disturbances $\Delta c_{A0} = 0.15\ \mathrm{kmol/m^3}$, $\Delta q_r = -0.03\ \mathrm{m^3/s}$ and $\Delta T_{r0} = 2\,\mathrm{K}$ were injected into nonlinear model of the reactor in times $t_v = 220\,\mathrm{s}$, $t_v = 440\,\mathrm{s}$ and $t_v = 640\,\mathrm{s}$. The controller parameters were estimated only in the first (tracking) interval $t < 200$ s. The authors' experiences proved that an utilization of recursive identification using the delta model after reaching of a constant reference and in presence of step disturbances decreases the control quality. From this reason, during interval $t \geq 200$ s, fixed parameters were used. The controlled output responses are shown in Fig. 9.

A preference of the 2DOF control system structure in comparison with the 1DOF structure with only feedback controller Q can be seen in Figs. 10 and 11. The use of the 1DOF structure leads to higher over/undershoots of the controlled output. Moreover, there exists expressive difference between control input changes. This fact can be important in control of some reactors where expressive input changes are undesirable.

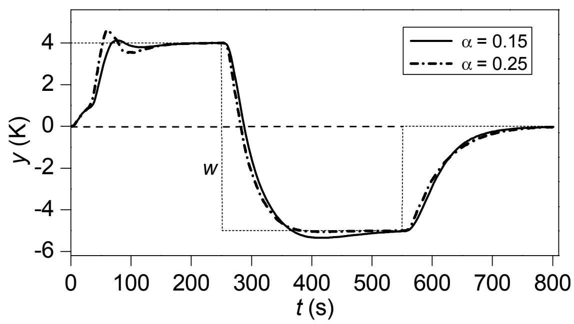

Fig. 6. Controlled output responses.

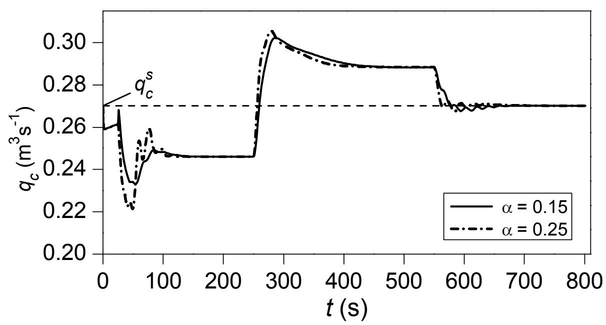

Fig. 7. Control input responses.

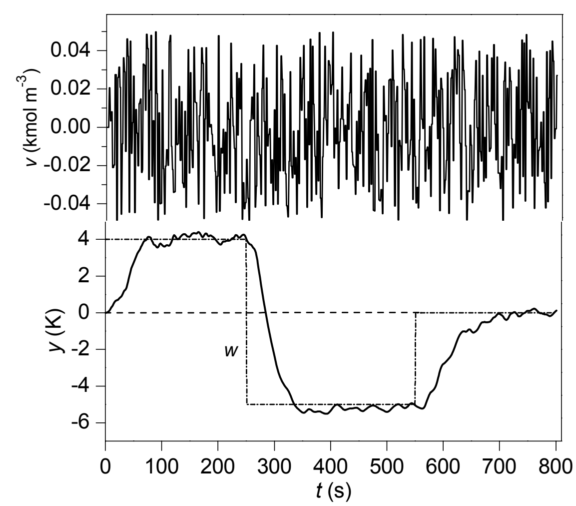

Fig. 8. Controlled output in the presence of unmeasured random disturbance in c_{A0} (α = 0.15)..

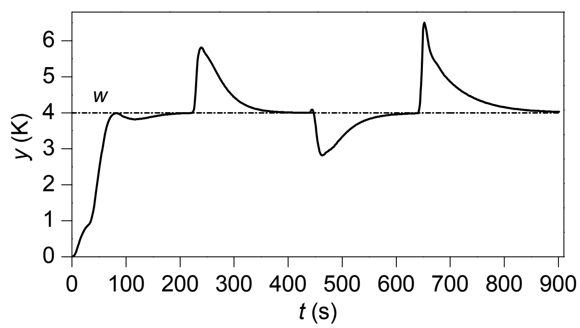

Fig. 9. Controlled output in the presence of step disturbances ($\alpha = 0.15$).

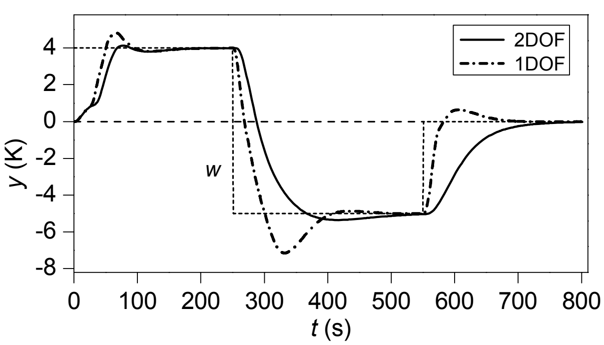

Fig. 10. Comparison of controlled outputs in the 1DOF and 2DOF structures ($\alpha = 0.15$).

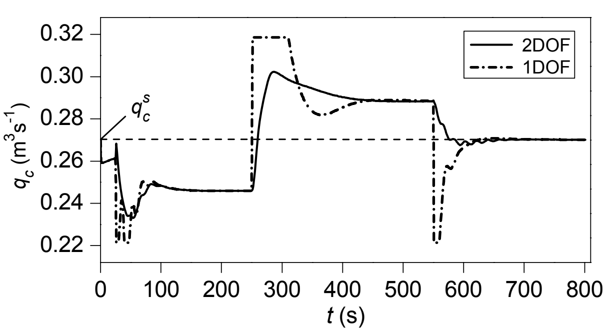

Fig. 11. Comparison of control inputs in the 1DOF and 2DOF structures ($\alpha = 0.15$).

IX. Conclusions

In this paper, one approach to the continuous-time adaptive control of the mean reactant temperature in a tubular chemical reactor was proposed. The control strategy is based on a preliminary analysis of the steady-state and dynamic analysis of the process behaviour and on the assumption of the temperature measurement along the reactor. The proposed algorithm employs an alternative continuous-time external linear model with parameters obtained through recursive parameter estimation of a corresponding delta model. The resulting continuous-time controller in the 2DOF control system structure is derived using the polynomial approach and given by a solution of two polynomial Diophantine equations. Tuning of its parameters is possible via closed-loop pole assignment. The presented method has been tested by computer simulation on the nonlinear model of the tubular chemical reactor with a consecutive exothermic reaction. Results demonstrate an applicability of the presented control strategy. It can be remarked that similar results have been obtained using the output temperature as the controlled output.

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