

# Decentralized Approach to a Control of Chemical Reactors

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An effective approach to the control of chemical reactors is described in this paper. The simplified theoretical mathematical model of two serially connected continuous-time stirred tank reactors is used for simulation of their dynamic properties. The control algorithm is based on having the input-output model of the controlled system. Such model is obtained by sampling of input and output variables and using one of recursive identification methods. Principles of decomposition are used to simplify the input-output model. Controller design uses the pole-placement method and principles of decentralization.

Chemical reactors constitute a major part of most chemical processing plants. Solution of the control problems of chemical reactors is connected with many difficulties. Some of them are very complicated mathematical models which describe various physical and chemical processes in reactors. To have proper models for control purposes, it is necessary to accept many simplifying assumptions. Other problems are caused by the usually nonlinear dynamics of chemical reactors. Some complications arise because of many internal interactions. The most important of them is the interaction between reaction temperature and reaction rate. For the control purposes, it is convenient to replace the theoretical mathematical model by a simplified external model, which describes the connection between the most important input and output variables. The coefficients of external model are usually obtained by recursive identification from measured inputs and outputs.

The goal of control consists *e.g.* in reaching the desired composition and temperature of reaction mixture, optimizing control time, ensuring safety processing, minimizing production expenses, *etc.* Today's industrial praxes prefer the stable state control [1, 2], when the safety processing can be ensured easily. From the economic point of view, the nonstable-state control can be more effective [1]. However, the more complicated control algorithms have to be used in this case. The advanced control algorithms are the adaptive ones based on input-output description of the controlled system, see *e.g.* Refs. [3, 4]. Some of them use principles of decomposition and decentralization [5]. These control algorithms present a group of algorithms, which enable to fulfil the control goals in a very attractive way. One of the last mentioned control algorithms is described in this paper.

## THEORETICAL

### Controlled System

Consider that the controlled system consists of two serially connected nonisothermal continuous-time stirred tank reactors (CTSTRs) with a recycle, as it is shown in Fig. 1. The first reactor is the CTSTR with the first-order irreversible parallel exothermic reactions according to the scheme  $A \xrightarrow{k_1} B$ ,  $A \xrightarrow{k_2} C$ . The second reactor is also a CTSTR with the first-order consecutive exothermic reactions according to the scheme  $B \xrightarrow{k_3} D \xrightarrow{k_4} E$ .  $k_1$ ,  $k_2$ ,  $k_3$ ,  $k_4$  are reaction rate coefficients which differ in their numerical values. The goal of the control is to reach the maximal production of the product D or to change the production in the surroundings of the maximum, so that the control time is shorter than the step response of the system. Under the condition of perfect mixing, the dynamic mathematical model of the entire system was obtained by mass balances of reactants, energy balance of the reactant mixture and energy balance

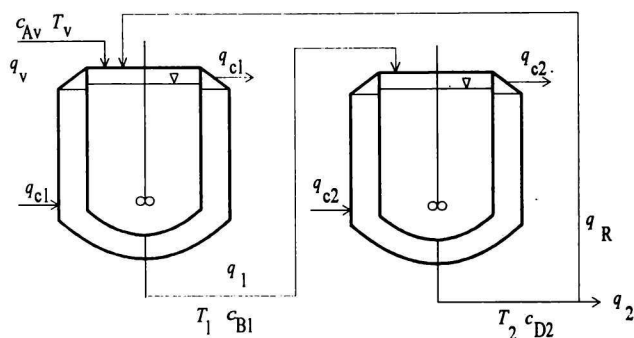


Fig. 1. Scheme of two serial chemical reactors with a recycle.

of the coolant. Many simplifications were accepted by modelling of considered reactors, so that the obtained model might be as simple as possible. Some of these simplifications are *e.g.* perfect mixing in the reactors, constant mass densities, volumes of reaction mixture, specific heat capacities, *etc.* The principles of obtaining models of chemical reactors proper for the control purposes are described *e.g.* in [1]. The nonlinear model of two serially connected chemical reactors with a recycle is described by fourteen differential equations in the form

1st reactor

$$\frac{dc_{A1}}{dt} = -(1/\tau_1 + k_1 + k_2)c_{A1} + (q_v c_{Av} + q_R c_{A2})/(\tau_1 q_1) \quad (1)$$

$$\frac{dc_{B1}}{dt} = -c_{B1}/\tau_1 + k_1 c_{A1} + q_R c_{B2}/(\tau_1 q_1) \quad (2)$$

$$\frac{dc_{C1}}{dt} = -c_{C1}/\tau_1 + k_2 c_{A1} + q_R c_{C2}/(\tau_1 q_1) \quad (3)$$

$$\frac{dc_{D1}}{dt} = -c_{D1}/\tau_1 + q_R c_{D2}/(\tau_1 q_1) \quad (4)$$

$$\frac{dc_{E1}}{dt} = -c_{E1}/\tau_1 + q_R c_{E2}/(\tau_1 q_1) \quad (5)$$

$$\frac{dT_1}{dt} = -T_1/\tau_1 + q_v T_v/(\tau_1 q_1) + \frac{Q_{R1} - Q_{C1}}{\tau_1 q_1 \rho_1 c_{p1}} + \frac{q_R \rho_2 c_{p2}}{\tau_1 q_1 \rho_1 c_{p1}} T_2 \quad (6)$$

$$\frac{dQ_{c1}}{dt} = -Q_{c1}/\tau_{c1} + \varphi_1(T_1 - T_{cv})/\tau_{c1} \quad (7)$$

2nd reactor

$$\frac{dc_{A2}}{dt} = -c_{A2}/\tau_2 + c_{A1} q_1 / ((q_2 + q_R) \tau_2) \quad (8)$$

$$\frac{dc_{B2}}{dt} = -(1/\tau_2 + k_3)c_{B2} + c_{B1} q_1 / ((q_2 + q_R) \tau_2) \quad (9)$$

$$\frac{dc_{C2}}{dt} = -c_{C2}/\tau_2 + c_{C1} q_1 / ((q_2 + q_R) \tau_2) \quad (10)$$

$$\frac{dc_{D2}}{dt} = -(1/\tau_2 + k_4)c_{D2} + c_{D1} q_1 / ((q_2 + q_R) \tau_2) + k_3 c_{B2} \quad (11)$$

$$\frac{dc_{E2}}{dt} = -c_{E2}/\tau_2 + k_4 c_{D2} + c_{E1} q_1 / ((q_2 + q_R) \tau_2) \quad (12)$$

$$\frac{dT_2}{dt} = -T_2/\tau_2 + \frac{Q_{R2} - Q_{C2}}{\tau_2 (q_2 + q_R) \rho_2 c_{p2}} + \frac{q_1 \rho_1 c_{p1}}{\tau_2 (q_2 + q_R) \rho_2 c_{p2}} T_1 \quad (13)$$

$$\frac{dQ_{c2}}{dt} = -Q_{c2}/\tau_{c2} + \varphi_2(T_2 - T_{cv})/\tau_{c2} \quad (14)$$

where

$$\tau_1 = V_1/q_1, \quad \tau_2 = V_2/(q_2 + q_R),$$

$$\tau_{c1} = \frac{V_{c1} \rho_c c_{pc}}{q_{c1} \rho_c c_{pc} + F_1 \alpha_1}, \quad \tau_{c2} = \frac{V_{c2} \rho_c c_{pc}}{q_{c2} \rho_c c_{pc} + F_2 \alpha_2} \quad (15)$$

$$\varphi_1 = \frac{q_{c1} \rho_c c_{pc} F_1 \alpha_1}{q_{c1} \rho_c c_{pc} + F_1 \alpha_1}, \quad \varphi_2 = \frac{q_{c2} \rho_c c_{pc} F_2 \alpha_2}{q_{c2} \rho_c c_{pc} + F_2 \alpha_2} \quad (16)$$

$$Q_{R1} = [(-\Delta H_1)k_1 + (-\Delta H_2)k_2]V_1 c_{A1},$$

$$Q_{R2} = [(-\Delta H_3)k_3 c_{B2} + (-\Delta H_4)k_4 c_{D2}]V_2 \quad (17)$$

The rates of reactions per volume unit for the 1st reactor are

$$r_1 = k_1 c_{A1}, \quad r_2 = k_2 c_{A1} \quad (18)$$

and for the 2nd one

$$r_3 = k_3 c_{B2}, \quad r_4 = k_4 c_{D2} \quad (19)$$

The rate coefficients  $k_i$  are nonlinear functions of reaction temperatures being described by the Arrhenius relation

$$k_i = k_{i0} \exp\left(-\frac{E_i}{RT_i}\right), \quad i = 1, 2, 3, 4 \quad (20)$$

The mathematical state model of the two reactors described above is then a system of fourteen nonlinear differential equations and the controller design of such a system by classical methods of the control theory would be very complicated. The model (1–14) is used only for simulation and obtaining of numerical values of its input and output variables instead of having a real process.

## CONTROLLER DESIGN

The approach described below is based on having the external model of the controlled process with several inputs and several outputs with predefined order of dynamics. In our case, the above described theoretical model is too complicated for finding a good controller. It is necessary to approximate it by any simpler model. One way how to solve the problem of simplification is to replace the theoretical model by an experimental external model which describes influence of measurable input variables on measurable system outputs, see *e.g.* [6]. In this case, it is necessary to predefine the number of inputs and outputs and also the sufficient order of dynamics. For the model (1–14), we suppose that controlled reactors are well described by the external model with two inputs  $u_1(k)$ ,  $u_2(k)$ , two outputs  $y_1(k)$ ,  $y_2(k)$ , and the second-order dynamics. Then, coolant flow rates in reactors were chosen as the inputs  $u_1(k)$ ,  $u_2(k)$  and temperatures of reaction mixtures in the individual reactors as the outputs  $y_1(k)$ ,  $y_2(k)$ .

The external mathematical model of the system with two inputs, two outputs, and the second-order dynamics is described by (see *e.g.* [6])

$$\begin{pmatrix} \delta^2 + a_1\delta + a_0 & a_3\delta + a_2 \\ a_5\delta + a_4 & \delta^2 + a_7\delta + a_6 \end{pmatrix} \begin{pmatrix} y_1(k) \\ y_2(k) \end{pmatrix} \\ = \begin{pmatrix} b_1\delta + b_0 & 0 \\ 0 & b_5\delta + b_4 \end{pmatrix} \begin{pmatrix} u_1(k) \\ u_2(k) \end{pmatrix} \quad (21)$$

where  $\delta$  is the difference operator defined by [6] so that

$$\delta y(k) = \frac{y(k+1) - y(k)}{T_s}, \quad \delta u(k) = \frac{u(k+1) - u(k)}{T_s} \\ \delta^2 y(k) = \frac{y(k+2) - 2y(k+1) + y(k)}{T_s^2}, \\ \delta^2 u(k) = \frac{u(k+2) - 2u(k+1) + u(k)}{T_s^2} \quad (22)$$

where  $k$  is the discrete time,  $T_s$  is the sampling period (time between two measurements on the process). The operator  $\delta y$  represents the difference of  $y$ ,  $\delta^2 y$  the second difference of  $y$ , and generally  $\delta^n y$  is the  $n$ -th difference of  $y$ . The inherent property of the operator (22) is that it converges to the continuous derivative operator as the sampling period tends to zero. Thus, the model (21) represents two second-order differential equations, when  $T_s \rightarrow 0^+$ . The model (21) is much simpler than that described by eqns (1–14) because of having two difference equations instead of fourteen differential ones. Thus, the model (21) is more proper for mathematical finding of a controller. The numerical values of parameters  $a_0, \dots, a_7, b_0, \dots, b_5$  are obtained by statistical analysis of sampled inputs  $u_1(k), u_2(k)$  and outputs  $y_1(k), y_2(k)$ .

The other advantage of this model consists in a possibility to decompose the system (21) in two subsystems. The first of them represents the first reactor and is described by

$$(\delta^2 + a_1\delta + a_0)y_1(k) + h_1(k) = (b_1\delta + b_0)u_1(k) \quad (23)$$

and the second one represents the second reactor and is described by

$$(\delta^2 + a_7\delta + a_6)y_2(k) + h_2(k) = (b_5\delta + b_4)u_2(k) \quad (24)$$

Variables  $h_1(k), h_2(k)$  are the interconnections defined as

$$h_1(k) = (a_3\delta + a_2)y_2(k) \quad (25)$$

$$h_2(k) = (a_5\delta + a_4)y_1(k) \quad (26)$$

and they express the mutual influence of reactors.

The principles of decomposition and decentralization have been used for controller design. The theoretical background and the derivation of the control

algorithm can be found *e.g.* in [7, 8]. Then, it is necessary to find such a control, which will be able to ensure desired goals of control. The decentralization approach supposes that the control of the  $i$ -th subsystem  $u_i(k)$  consists of two parts

$$u_i(k) = u_i^l(k) + u_i^g(k) \quad (27)$$

The first of them is called the local control  $u_i^l(k)$  and controls the isolated subsystem. The second part is called the global control  $u_i^g(k)$  and compensates the influence of interconnections.

### Local Control

The design of local control is based on polynomial approach in continuous-time domain, see *e.g.* [9, 10]. Let each of decomposed isolated subsystems be modelled by eqns (23), (24) with  $h_1 = 0, h_2 = 0$ . Further consider the step changes of reference values  $w_1, w_2$  and the local control loop with two controllers with their transfer functions

$$\frac{q(\delta)}{p(\delta)} = \frac{q_{1i}\delta + q_{0i}}{p_{1i}\delta + p_{0i}}, \quad \frac{r(\delta)}{p(\delta)} = \frac{r_{0i}}{p_{1i}\delta + p_{0i}}, \quad i = 1, 2 \quad (28)$$

where  $p(\delta), q(\delta), r(\delta)$  are polynomials in  $\delta$  and  $q_{1i}, q_{0i}, p_{1i}, p_{0i}, r_{0i}$  are coefficients, which have to be found. Then, the synthesis equations for the first subsystem have the form (see [9, 10])

$$\begin{aligned} &(\delta^2 + a_1\delta + a_0)(p_{11}\delta + p_{01}) \\ &+ (b_1\delta + b_0)(q_{11}\delta + q_{01}) \\ &= \delta^3 + d_2\delta^2 + d_1\delta + d_0 \end{aligned} \quad (29)$$

$$\begin{aligned} &\delta(t_{21}\delta^2 + t_{11}\delta + t_{01}) + (b_1\delta + b_0)r_{01} \\ &= \delta^3 + d_2\delta^2 + d_1\delta + d_0 \end{aligned} \quad (30)$$

where  $(t_{21}\delta^2 + t_{11}\delta + t_{01})$  is an auxiliary polynomial and  $\delta^3 + d_2\delta^2 + d_1\delta + d_0$  is polynomial, which has to be chosen properly, see *e.g.* [4]. The choice of coefficients on the right sides of eqns (29), (30) determines the dynamic behaviour of the control loop. The parameters of controllers (28) are calculated from (29), (30). Then, the local control law of the first subsystem can be described by

$$\begin{aligned} u_1^l(k) &= [(p_{11} - p_{01}T_s)u_1^l(k-1) + r_{01}T_s w_1(k-1) \\ &- q_{11}y_1(k) + (q_{11} - q_{01}T_s)y_1(k-1)]/p_{11} \end{aligned} \quad (31)$$

Similarly, the local control law of the second subsystem is

$$\begin{aligned} u_2^l(k) &= [(p_{12} - p_{02}T_s)u_2^l(k-1) + r_{02}T_s w_2(k-1) \\ &- q_{12}y_2(k) + (q_{12} - q_{02}T_s)y_2(k-1)]/p_{12} \end{aligned} \quad (32)$$

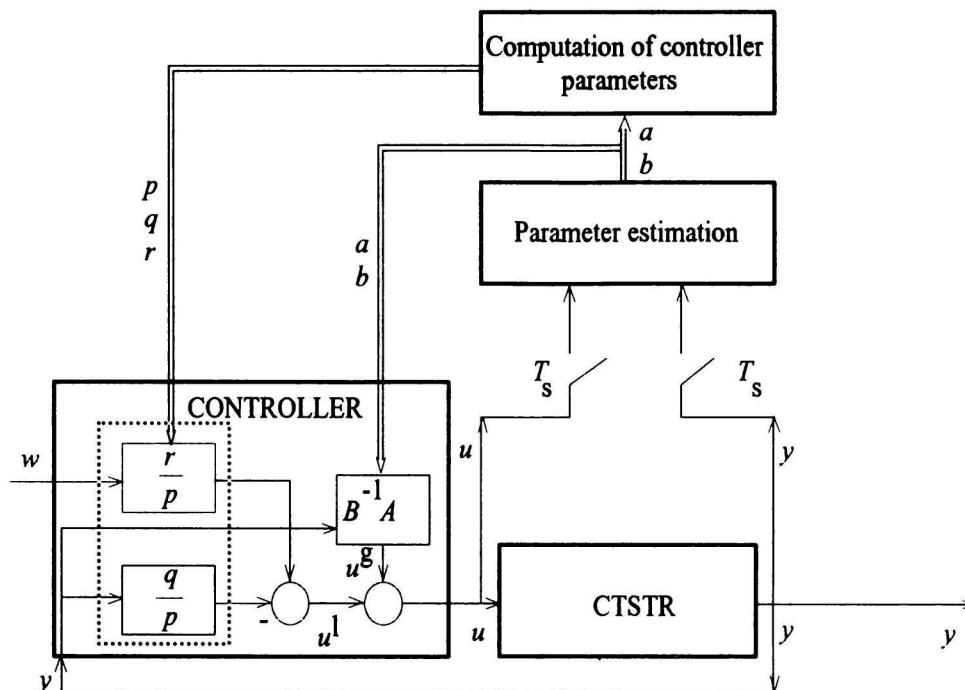


Fig. 2. Adaptive control loop.

Table 1. Parameter Values Used for Simulation

$q_v = 0.32 \text{ m}^3 \text{ min}^{-1}$	$V_1 = 1.2 \text{ m}^3$	$V_2 = 1.2 \text{ m}^3$
$q_R = 0.03 \text{ m}^3 \text{ min}^{-1}$	$F_1 = 5.6 \text{ m}^2$	$F_2 = 5.6 \text{ m}^2$
$q_1 = 0.35 \text{ m}^3 \text{ min}^{-1}$	$\rho_1 = 802 \text{ kg m}^{-3}$	$\rho_2 = 796 \text{ kg m}^{-3}$
$q_2 = 0.32 \text{ m}^3 \text{ min}^{-1}$	$c_{p1} = 3.97 \text{ kJ kg}^{-1} \text{ K}^{-1}$	$c_{p2} = 3.94 \text{ kJ kg}^{-1} \text{ K}^{-1}$
$c_{Av} = 9.82 \text{ kmol m}^{-3}$	$\alpha_1 = 38.9 \text{ kJ m}^{-2} \text{ min}^{-1} \text{ K}^{-1}$	$\alpha_2 = 41.2 \text{ kJ m}^{-2} \text{ min}^{-1} \text{ K}^{-1}$
$T_v = 328 \text{ K}$	$k_{10} = 6.219 \times 10^{12} \text{ min}^{-1}$	$k_{30} = 2.703 \times 10^8 \text{ min}^{-1}$
$\rho_c = 998 \text{ kg m}^{-3}$	$k_{20} = 1.262 \times 10^{26} \text{ min}^{-1}$	$k_{40} = 2.223 \times 10^{27} \text{ min}^{-1}$
$c_{pc} = 4.182 \text{ kJ kg}^{-1} \text{ K}^{-1}$	$E_1/R = 10032 \text{ K}$	$E_3/R = 6896 \text{ K}$
$V_{c1} = V_{c2} = 0.64 \text{ m}^3$	$E_2/R = 20672 \text{ K}$	$E_4/R = 23453 \text{ K}$
$T_{cv} = 293 \text{ K}$	$(-\Delta H_1) = 1750 \text{ kJ kmol}^{-1}$	$(-\Delta H_3) = 10500 \text{ kJ kmol}^{-1}$
$T_s = 0.5 \text{ min}$	$(-\Delta H_2) = 12800 \text{ kJ kmol}^{-1}$	$(-\Delta H_4) = 7500 \text{ kJ kmol}^{-1}$

## Global Control

The global parts of subsystem control were determined so that they are able to compensate the influence of interconnections between subsystems. The following equations hold for the first and for the second subsystem

$$(a_3\delta + a_2)y_2(k) = (b_1\delta + b_0)u_1^g(k) \quad (33)$$

$$(a_5\delta + a_4)y_1(k) = (b_5\delta + b_4)u_2^g(k) \quad (34)$$

Eqns (33) and (34) represent generally a system of difference equations which must be solved along with the control law. These equations can be transformed in algebraic equations at the conditions  $\delta u(k) = 0$  and  $\delta y(k) = 0$  in the steady state. Under this simplifying condition, it is possible to obtain the global parts of control in the form

$$A \begin{pmatrix} y_2(k) \\ y_1(k) \end{pmatrix} = B \begin{pmatrix} u_1^g(k) \\ u_2^g(k) \end{pmatrix} \quad (35)$$

where  $A = \begin{pmatrix} a_2 & 0 \\ 0 & b_4 \end{pmatrix}$ ,  $B = \begin{pmatrix} b_0 & 0 \\ 0 & b_4 \end{pmatrix}$  and then

$$\begin{pmatrix} u_1^g(k) \\ u_2^g(k) \end{pmatrix} = B^{-1}A \begin{pmatrix} y_2(k) \\ y_1(k) \end{pmatrix} \quad (36)$$

## RESULTS

The algorithm described above was implemented for simulation purposes in the adaptive form. The adaptive control loops are described *e.g.* in [11, 12]. The block scheme of an adaptive control loop is shown in Fig. 2. Instead of having the real process, the mathematical model (1–14) was simulated on a PC. Then, the input variables (coolant flow rates) and the output ones (temperatures of reaction mixtures) were sampled with predefined sampling period  $T_s$ . These data were stored in a memory and used for identification

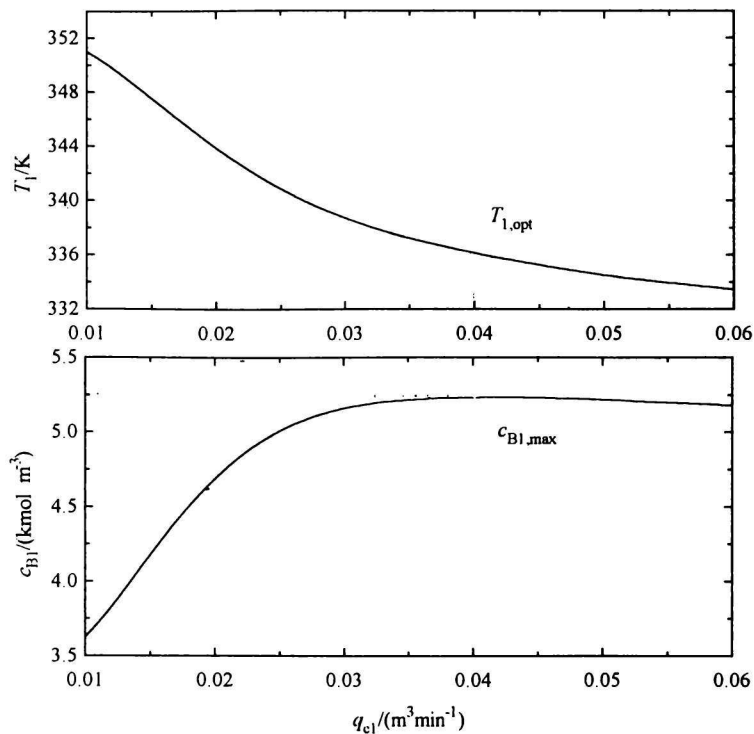


Fig. 3. Steady-state dependence of  $c_{B1}$ ,  $T_1$  on  $q_{c1}$ .

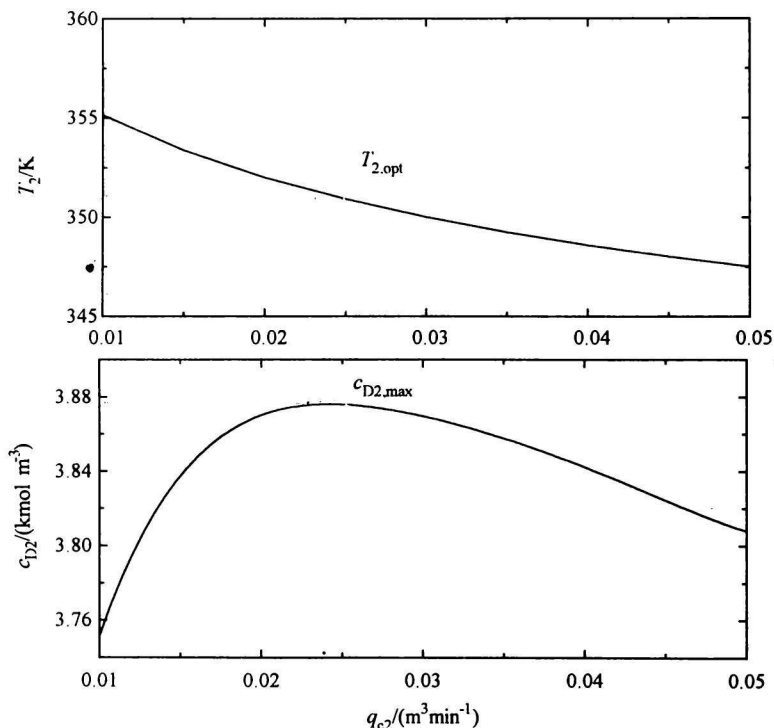


Fig. 4. Steady-state dependence of  $c_{D2}$ ,  $T_2$  on  $q_{c2}$ .

of parameters of the external model (21). The adaptive algorithm required to evaluate these parameters in each sampling period, when the new values of input and output variables were added. So one of the

recursive identification methods (REFIL, LDFIL, LDDIF) had to be used. Presented control algorithm uses the recursive identification method LDDIF (see e.g. [9]) based on the least-squares method. The recur-

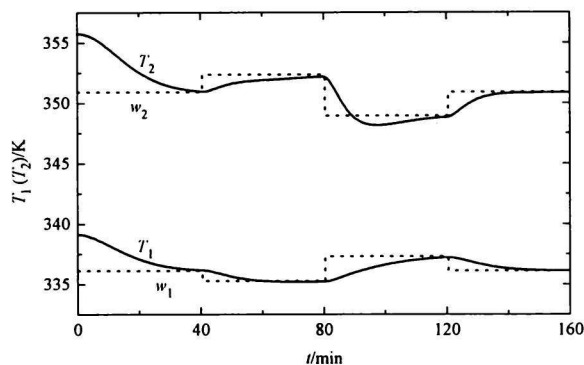


Fig. 5. Step responses of the CTSTR – output variables.

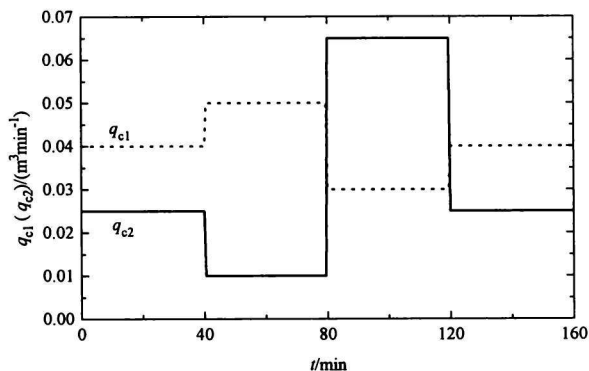


Fig. 6. Step responses of the CTSTR – input variables.

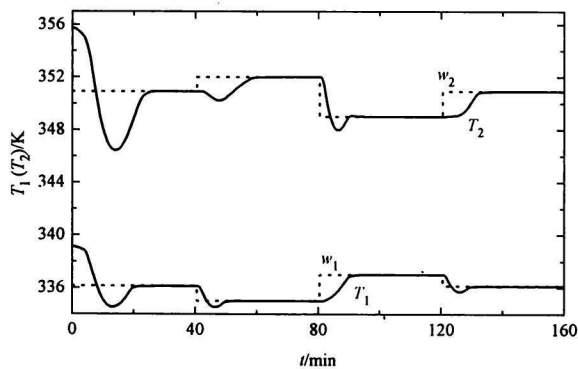


Fig. 7. Control responses of the CTSTR – output variables and references.

sive identification enabled to take changes of output and input variables into account. After the parameters of external model were calculated, the parameters of controllers could be evaluated and control laws could be calculated by eqns (31), (32), (36) and so the PC served as a self-tuner, which realized the control laws.

The parameters used for simulation are in Table 1. These parameters describe theoretical reaction system and serve only for simulation. The analysis of the static behaviour of the system of two serial CTSTRs shows (Figs. 3 and 4) that the optimal working points of the system are temperatures  $T_{1,opt} = 336.1$  K in

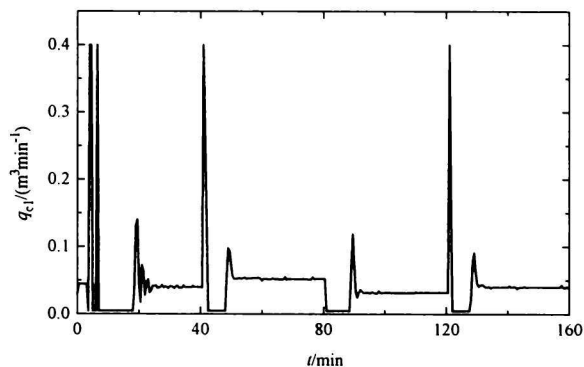


Fig. 8. Control responses of the CTSTR – input variable in the first reactor.

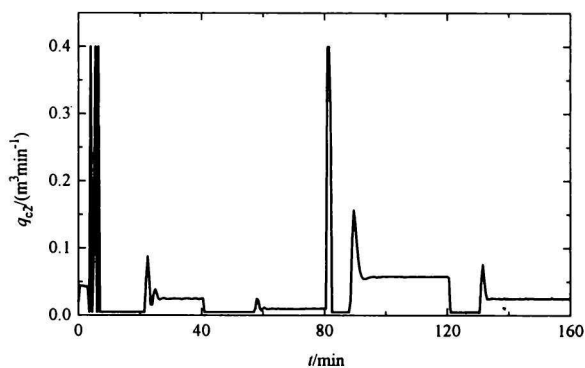


Fig. 9. Control responses of the CTSTR – input variable in the second reactor.

the first reactor and  $T_{2,opt} = 350.9$  K in the second reactor. These temperatures were reached, when the coolant flow rate in the first reactor was  $0.04 \text{ m}^3 \text{ min}^{-1}$  and in the second one  $0.025 \text{ m}^3 \text{ min}^{-1}$ . At these conditions a maximal concentration of the product D  $c_{D2,max}$  could be achieved.

To compare the dynamic behaviour of the uncontrolled and controlled systems, the step responses of the CTSTR were obtained at first and they are shown in Figs. 5 and 6. These step responses exhibited overdamped dynamics and it took about 40 min to reach a new steady state. The control responses of the CTSTR are shown in Figs. 7–9. The controlled outputs reach their set points  $w_1, w_2$  after less than 20 min. For the reason of occurring many industrial boundaries the inputs in the controlled system were limited into the interval  $(0; 0.4 \text{ m}^3 \text{ min}^{-1})$ .

## CONCLUSION

It is very important from the viewpoint of its industrial utilization to have a good control algorithm for chemical processing plants. The control algorithm designed in the presented paper has several advantages. It does not require to have an exact mathematical model of the controlled process. The external

input-output model can be obtained by the measurement of the input and output variables and the use of some of the recursive identification methods. Having the real process, the inputs and outputs can be measured on it. For these purposes it is not necessary to know the reaction kinetics exactly. The investigated control algorithm is adaptive and the controller parameters vary as some properties of the controlled system change. Presented control algorithm is also very simple as it is based on the decomposition and decentralization approaches. The local and global controls are very simple and the entire control is only the sum of two previous ones. The convergence properties of the proposed algorithm are very good, too, and realistic simulations demonstrate convenience of using delta operators. The formulation and implementation of delta model self-tuning controllers do not bring any additional problems and difficulties.

## SYMBOLS

$c_A, c_B, c_C, c_D$	reactant concentrations	$\text{kmol m}^{-3}$
$t$	time	min
$k_1, k_2, k_3, k_4$	reaction rate coefficients	$\text{min}^{-1}$
$c_{Av}$	feed concentration	$\text{kmol m}^{-3}$
$q, q_c, q_R$	volumetric flow rates	$\text{m}^3 \text{min}^{-1}$
$q_v$	feed volumetric flow rate	$\text{m}^3 \text{min}^{-1}$
$Q_R$	reaction heat	$\text{kJ min}^{-1}$
$Q_c$	heat accepted by coolant	$\text{kJ min}^{-1}$
$\rho, \rho_c$	reactant and coolant densities	$\text{kg m}^{-3}$
$c_p, c_{pc}$	specific heat capacities	$\text{kJ kg}^{-1}\text{K}^{-1}$
$T, T_c$	reactant and coolant temperatures	K
$T_v, T_{cv}$	feed values for $T$ and $T_c$	K
$V, V_c$	reactant and coolant volumes	$\text{m}^3$
$F$	heat exchange surface area	$\text{m}^2$
$\alpha$	heat transfer coefficient	$\text{kJ m}^{-2}\text{min}^{-1}\text{K}^{-1}$
$(-\Delta H_1), (-\Delta H_2), (-\Delta H_3), (-\Delta H_4)$	specific reaction heats	$\text{kJ kmol}^{-1}$
$r_1, r_2, r_3, r_4$	reaction rates	$\text{kmol m}^{-3} \text{min}^{-1}$
$E_1, E_2, E_3, E_4$	activation energies	$\text{kJ kmol}^{-1}$

$k_{10}, k_{20}, k_{30}, k_{40}$	Arrhenius preexponential constants	$\text{min}^{-1}$
$R$	gas constant	$\text{kJ kmol}^{-1} \text{K}^{-1}$
$k$	discrete time	
$u$	control input	$\text{m}^3 \text{min}^{-1}$
$y$	controlled output	K
$\delta$	discrete time operator	
$T_s$	sampling period	min
$w$	reference signal	

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