Robust control of a chemical reactor with uncertainties

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Abstract: This work deals with the design and the application of a robust control to a chemical reactor. The reactor is exothermic one. There are two parameters with only approximately known values in the reactor. These parameters are the reaction enthalpies. Because of the presence of uncertainty, the robust output feedback is designed. Two robust controllers are designed, the first one is based on the small gain theorem and the second one uses the H_2/H_∞ control techniques. The presented experimental results confirm applicability of mentioned approaches to safe control of nonlinear processes.

Keywords: exothermic chemical reactor, robust control, small gain theorem, H_2/H_∞ control

Introduction

In this paper the small gain theorem and the H_2/H_∞ control techniques are applied to control of a chemical reactor.

It is well known that the control of chemical reactors represents very complex problem (Luyben 2007; Molnár et al. 2002). Continuous stirred tank reactors (CSTRs) are often used plants in chemical industry and especially exothermic CSTRs are very interesting systems from the control viewpoint (Bequette 1991). The dynamic characteristics may exhibit e.g. a varying sign of the gain in various operating points, the time delay or the non-minimum phase behaviour. Various types of disturbances also affect operation of chemical reactors, operation of chemical reactors is corrupted by different uncertainties. Some of them arise from varying or not exactly known parameters, as e.g. reaction rate constants, reaction enthalpies or heat transfer coefficients (Antonelli and Astolfi 2003). All these problems can cause poor control response or even instability of classical closed-loop control systems.

Effective control of CSTRs requires application of some of advanced methods, as e. g. robust control (Gerhard et al. 2004; Tlacuahuac et al. 2005). Robust control has grown as one of the most important areas in the modern control design since works by (Doyle 1981; Zames 1983) and many others.

The classical small-gain theorem (Green and Limebeer 1994) is an important tool for analyzing the input-output stability of feedback systems and the tool for robust controller design for systems with unstructured uncertainty (Nešić and Liberzon 2005; Karafyllis and Zhong-Ping 2007). Some nonlinear versions of the classical small-gain theorem are derived for input-output stability of nonlinear feedback systems. The notion of input-to-state stability (ISS) was originally introduced by Sontag (Sontag 1989). Following this, a nonlinear, generalized small-gain theorem was developed (Jiang et al. 1996). Stability of interconnections of ISS systems has been studied by many authors (Laila and Nešić, 2003; Chaves 2005; Teel 2005; Angeli and Astolfi 2007; Ito 2008).

H_2 and H_∞ control theories have been active areas of research for the years and have been successfully introduced to many engineering applications. H_2 – optimization finds a controller which minimizes the H_2 norm of the closed-loop transfer function and internally stabilizes the system. The closed-loop transfer function to be minimized is located between the external signal and the control error signal (Kučera 2008). The polynomial solution of the standard H_2 problem is proposed e.g. in (Henrion et al. 2005; Kučera 2007; Yang et al. 2007). There exist various solutions also of the standard H_∞ problem. While the H_2 norm of a signal is the mean energy with respect to the frequency, the H_∞ norm is the maximum energy with respect to the frequency. If there are uncertainties in the system model, some quantity combining the H_2 norm and the H_∞ norm can be a desirable measure of a system's robust performance. Thus the mixed H_2/H_∞ performance criterion provides an interesting measure for the controller evaluation. The theoretic motivation for the mixed H_2/H_∞ control problem has been discussed in ((Doyle 1984; Kwakernaak 2002; Scherer 2006).

In the presented paper, the small gain theorem and the mixed H_2/H_∞ control theory with pole-placement are applied to robust controller design.

Small gain theorem

Suppose that the transfer function of an uncertain continuous-time system with additive unstructured uncertainty has the form

$$G(s) = G_n(s) + G_{\Delta a}(s) = G_n(s) + W_a(s)\Delta_a(s) \tag{1}$$

where $G_n(s)$ is the nominal model, $W_a(s)$ is the weight function and $\Delta_a(s)$ is a category of uncertainties that satisfies the condition $|\Delta_a(j\omega)| \leq 1$ for $\forall\omega$.

The task is to find a robust controller for control of the system (1). The design method is based on the small gain theorem (Green and Limebeer 1994; Veselý and Harsanyi 2007) and uses the fact that if a feedback loop consists of a stable systems and the loop-gain product is less than unity, then the feedback loop is internally stable. The other basis for the design is a fixed point theorem known as the contraction mapping theorem (Khalil 1996).

According to the small gain theorem, following conditions have to be satisfied: the controller with the transfer function $C(s)$ stabilizes the nominal model and for the open-loop transfer function $L(s)$, the condition given in (2) also holds.

$$L(s) = G(s)C(s),\ |L(j\omega)| < 1 \tag{2}$$

The family of the controlled system transfer functions $G(s)$ creates a set, in which $G_n(s)$ is the transfer function of the nominal system and $G_k(s)$ is a transfer function from the set $G(s)$, which differs from $G_n(s)$. Then, the value $l_a(\omega)$ can be calculated as the maximal value of modules as it is shown in (3)

$$l_a(s) = \max|G_k(j\omega) - G_n(j\omega)|,$$

$$\omega \in (0, \infty),\ k = 1, 2... \tag{3}$$

The characteristic equation of the closed loop with the uncertain controlled system is

$$1 + G(s)C(s) = 0 \tag{4}$$

and after the substitution (1) into (4), we obtain

$$[1 + G(s)\,C(s)]\left[1 + T_0(s)\frac{G_{\Delta a}(s)}{G_n(s)}\right] = 0 \tag{5}$$

where $T_0(s)$ is the closed-loop transfer function with the nominal model and has the form

$$T_0(s) = \frac{G_n(s)\,C(s)}{1 + G_n(s)\,C(s)} \tag{6}$$

The closed loop must be stable. The small gain theorem requires satisfying also the second condition. It follows from (5) that for the second term in (5) the following condition holds

$$\left[1 + T_0(s)\frac{G_{\Delta a}(s)}{G_n(s)}\right] = 0 \tag{7}$$

Then after the substitution $s = j\omega$ we obtain

$$\left|T_0(j\omega)\frac{G_{\Delta a}(j\omega)}{G_n(\omega)}\right| < 1, \forall\omega \in (0, \infty) \tag{8}$$

The conditions $|\Delta_a(j\omega)| = 1$ and $|W_a(j\omega)| = l_a(\omega)$ represent the worst cases and so, it is possible to rewritten (8) to the form

$$|T_0(j\omega)| < \frac{|G_n(j\omega)|}{l_a(\omega)} \tag{9}$$

Robust controller design is then based on finding parameters of the transfer function $T_0(s)$, the choice of the structure of the robust controller and calculation of the controller parameters.

Mixed H_2/H_∞ control synthesis

The role of H_∞ is to minimize the disturbance effect on the system output whereas H_2 is used to improve the transients against random disturbances.

Consider the plant model with the feedback as shown in Figure 1 (Bosgra and Kwakernaak 2000). The signal w represents the external input, z is the error of control, u is the manipulated variable vector, and y is the measured output. The block G is the generalised controlled process, and C is the compensator.

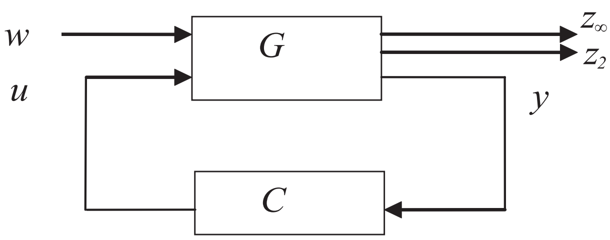

Fig. 1. Standard control configuration.

The loop gain has a direct effect on important closed-loop transfer functions which determine the norm, such as the sensitivity S and the complementary sensitivity T. The sensitivity and the complementary sensitivity functions are given by

$$\begin{aligned} S &= (I + GC)^{-1} \\ T &= (I + GC)^{-1}GC \end{aligned} \tag{10}$$

The H_2/H_∞ problem represents finding a controller C which minimizes the mixed H_2/H_∞ criterion

$$\mu||T_\infty||^2_\infty + \eta||T_2||^2_2 \tag{11}$$

where, $T_\infty(s)$ and $T_2(s)$ denote the closed-loop transfer functions from w to z_∞ and z_2, respectively, μ and η are scalar factors.

Assume G has realization

$$\begin{aligned} \dot{x} &= Ax + B_1 w + B_2 u \\ z_\infty &= C_\infty x + D_{\infty 1} w + D_{\infty 2} u \\ z_2 &= C_2 x + D_{21} w + D_{22} u \\ y &= C_y x + D_{y1} w + D_{y2} u \end{aligned} \tag{12}$$

where z_∞ is the output associated with the H_∞ performance, z_2 is the output associated with the H_2 performance (with the LQG aspects).
Let the closed-loop equations be

$$\begin{aligned} \dot{x}_{cl} &= A_{cl}x_{cl} + B_{cl}w \\ z_\infty &= C_{cl\infty}x_{cl} + D_{cl\infty}w \\ z_2 &= C_{cl2}x_{cl} + D_{cl2}w \end{aligned} \tag{13}$$

The closed-loop transfer functions $T_\infty(s)$ and $T_2(s)$ are

$$\begin{aligned} T_2(s) &= C_{cl2}(sI - A_{cl})^{-1}B_{cl} + D_{cl2} \\ T_\infty(s) &= C_{cl\infty}(sI - A_{cl})^{-1}B_{cl} + D_{cl\infty} \end{aligned} \tag{14}$$

H_∞ performance
Lemma 1: The closed-loop random Mean Square (RMS) gain for $T_\infty(s)$ does not exceed γ if and only if there exists a symmetric matrix such that (Chilali and Gahinet 1996; Scherer et al. 1997):

$$\begin{pmatrix} A_{cl}X_\infty + X_\infty A_{cl}^T \, B_{cl} \, X_\infty C_{cl\infty}^T \\ B_{cl\infty}^T - ID_{cl\infty}^T \\ C_{cl\infty}X_\infty D_{cl\infty} - \gamma^2 I \end{pmatrix} < 0, x_\infty > 0 \tag{15}$$

H_2 performance
Lemma 2: The closed-loop H_2-norm of $T_2(s)$, $||T_2||_2^2 = tr(C_{cl2}x_2C_{cl2}^T)$, does not exceed ν if and only $D_{cl2} = 0$ and there exist two symmetric matrices $X_2 > 0$ and Q such that (Chilali and Gahinet 1996; Scherer et al. 1997):

$$\begin{aligned} &\begin{pmatrix} A_{cl}X_2 + X_2A_{cl}^T B_{cl} \\ B_{cl}^T - I \end{pmatrix} < 0, \\ &\begin{pmatrix} QC_{cl2}X_2 \\ X_2C_{cl}^TX_2 \end{pmatrix} > 0, tr(Q) < \nu_2 \end{aligned} \tag{16}$$

The H_2 and the H_∞-norm are objectives that mutually compete, therefore a controller is found by solving (10), restricted to the former LMIs constraints:

$$\text{minimize } ||W_1S||_2 \text{ subject to } ||W_2T||_\infty < \gamma_\infty \tag{17}$$

Simulations and results

Consider a continuous-time stirred tank reactor (CSTR) with the first order irreversible parallel exothermic reactions according to the scheme

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

where B is the main product and C is the side product (Ingham et al. 1994; Vasičkaninová and Bakošová 2009; Vasičkaninová et al. 2011). The dynamic mathematical model of the reactor is obtained by mass balances of reactants, enthalpy balance of the reactant mixture and enthalpy balance of the coolant. Assuming ideal mixing in the reactor and the other usual simplifications, the simplified nonlinear dynamic mathematical model of the chemical reactor constitute four differential equations

$$\frac{dc_A}{dt} = \frac{q}{V}c_{Av} - \frac{q}{V}c_A - k_1c_A - k_2c_A \tag{18}$$

$$\frac{dc_B}{dt} = \frac{q}{V}c_{Bv} - \frac{q}{V}c_B + k_1c_A \tag{19}$$

$$\frac{dT}{dt} = \frac{q}{V}T_v - \frac{q}{V}T - \frac{Ak}{V\acute{A}c_p}(T - T_c) - \frac{h_1k_1 + h_2k_2}{\acute{A}cp}c_A \tag{20}$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c}T_{vc} - \frac{q_c}{V_c}T_c + \frac{Ak}{V_c\acute{A}_cc_{pc}}(T - T_c) \tag{21}$$

The reaction rate coefficients are the non-linear functions of the reaction temperature being defined by the Arrhenius relations

$$k_i = k_{i0}e^{-\frac{E_i}{RT}}, i = 1, 2 \tag{22}$$

In (18) – (22), c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, q are volumetric flow rates, h are reaction enthalpies, A is the heat transfer area, k_i is the heat transfer coefficient, k_{i0} is the pre-exponential factor, E is the activation energy and R is the universal gas constant. The subscript c denotes the coolant, the subscript v denotes the input and the superscript s denotes the steady-state values in the main operating point. The values of constant parameters and steady-state inputs of the chemical reactor are summarized in Table 1. Model uncertainty of the over described reactor follows from the fact that there are two physical parameters in this reactor, the reaction enthalpies, which values are known within following intervals (Table 2). The nominal values of these parameters are mean values of theirs intervals.
The reactions in the described reactor are exothermic ones and the heat generated by the chemical reactions is removed by the coolant in the jacket of the tank. The measured output is the temperature of the reaction mixture T, the coolant flow rate q_c is chosen as the control input.
The open-loop behaviour of the reactor was also studied using the data given in Table 1 and Table 2. Because of the presence of uncertainties, the reacting mixture temperatures obtained for the nominal model and also for 4 vertex systems are shown in Figure 2, 0 – nominal system, 1 – h_{1min}, h_{2min}, 2 – h_{1max},, h_{2max}, 3 – h_{1max}, h_{2min}, 4 – h_{1min}, h_{2max}.

Tab. 1. Constant parameters and steady-state inputs of the chemical reactor.

Variable	Unit	Value
q	$m^3 min^{-1}$	0.015
V	m^3	0.23
V_c	m^3	0.21
ρ	kg m^{-3}	1020
ρ_c	kg m^{-3}	998
c_p	kJ kg^{-1} K^{-1}	4.02
c_{pc}	kJ kg^{-1} K^{-1}	4.182
A	m^2	1.51
k	kJ m^{-2} min^{-1} K^{-1}	42.8
k_{10}	min^{-1}	1.55×10^{11}
k_{20}	min^{-1}	4.55×10^{25}
E_1/R	K	9850
E_2/R	K	22019
c_{Av}	kmol m^{-3}	4.22
c_{Bv}	kmol m^{-3}	0
c_{Cv}	kmol m^{-3}	0
T_v	K	328
T_{vc}	K	298
q^s_c	m^3 min^{-1}	0.004
T^s	K	363.61
T^s_c	K	350.15
c^s_A	kmol m^{-3}	0.4915
c^s_B	kmol m^{-3}	2.0042
c^s_C	kmol m^{-3}	1.7243

Tab. 2. Uncertain parameters of the chemical reactor.

Variable	Unit	Value
$-h_{1min}$	kJ $kmol^{-1}$	8.4×10^4
$-h_{1max}$	kJ $kmol^{-1}$	8.8×10^4
$-h_{2min}$	kJ $kmol^{-1}$	1.62×10^4
$-h_{2max}$	kJ $kmol^{-1}$	2.02×10^4

Robust controller design based on the small gain theorem

A robust PID controller was designed for control of the reaction mixture temperature. The transfer functions for the nominal system and 4 vertex systems are found for the step change of the coolant flow rate q_c from 0.004 m^3 min^{-1} to 0.008 m^3 min^{-1}:

$$G_n(s) = \frac{-1290}{85.184s^3 + 58.08s^2 + 13.2s + 1} \quad (23)$$

$$G_1(s) = \frac{-1580}{125s^3 + 75s^2 + 15s + 1} \quad (24)$$

$$G_2(s) = \frac{-1030}{216s^3 + 108s^2 + 18s + 1} \quad (25)$$

$$G_3(s) = \frac{-1400}{91.125s^3 + 60.75s^2 + 13.5s + 1} \quad (26)$$

$$G_4(s) = \frac{-1200}{103.82s^3 + 66.27s^2 + 14.1s + 1} \quad (27)$$

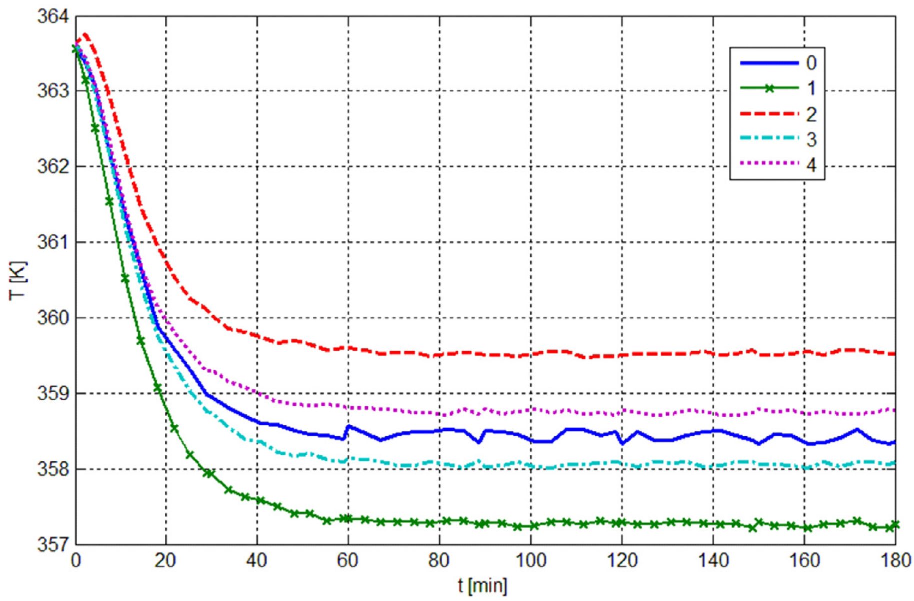

Fig. 2. Open-loop response of the CSTR – the reacting mixture temperature: 0 – nominal system, 1, 2, 3, 4 – vertex systems.

The transfer function $T_0(s)$ is in the form

$$T_0(s) = \frac{G_{nnum}(s)}{G_{nnum}(s) + D_{nden}(s)\, rs} \quad (28)$$

The controller transfer function has the structure

$$C(s) = \frac{C_{num}(s)}{C_{den}(s)} = \\ = \frac{1}{r}\frac{c_2 s^2 + c_1 s + c_0}{s} = P + \frac{I}{s} + Ds \quad (29)$$

The parameter r is an optional parameter and the function $T_0(s)$ has to satisfy (9). The polynomial $D_{n\,den}(s)$ is optional, too, and the following equation has to be satisfied

$$G_{n\,den}(s) = D_{n\,den}(s)C(s) \quad (30)$$

Unknown parameters are $d_1 = 4.4$, $c_2 = 19.36$, $c_1 = 8.8$, $c_0 = 1$ and they are calculated from

$$85.184s^3 + 58.08s^2 + 13.2s + 1 = \\ = (d_1 s + 1)(c_2 s^2 + c_1 s + c_0) \quad (31)$$

The transfer function $T_0(s)$ is affected by the choice of the parameter r and has the form

$$T_0(s) = \frac{1}{d_1 rs^2 + rs + 1} \quad (32)$$

The choice of r depends on the control signals boundaries, too. In Figure 3 the reference trajectory and the reacting mixture temperature obtained using the PID controller with parameters $r = 500$, $P = -1.76 \times 10^{-2}$, $I = -2.0 \times 10^{-3}$, $D = -3.87 \times 10^{-2}$ for the nominal model and also for 4 vertex systems are shown. Here, 0 is the nominal system and the vertex systems are the following combinations: 1 – h_{1min}, h_{2min}, 2 – h_{1max}, h_{2max}, 3 – h_{1max}, h_{2min}, 4 – h_{1min}, h_{2max}.

Figure 3 presents the set-point tracking and the disturbance rejection in the reactor. The disturbances were represented by the feed temperature changes of the reaction mixture. Following load disturbances were supposed: the feed temperature for the reaction mixture decreased by 5 K at $t = 100$ min, increased by 3 K at $t = 300$ min, decreased by 6 K at $t = 500$ min.

Figure 4 presents the control signal for the set-point tracking and the disturbance rejection.

H_2/H_∞ control

The transfer function describing the nominal system was supposed for the controller order reduction in the form (33) with parameters: $K = -1266$, $T = 7$ min, $n = 2$. These parameters were used for the H_2/H_∞-controller tuning.

$$G(s) = \frac{K}{(Ts+1)^n} \quad (33)$$

The controller was found in the form

$$C(s) = \frac{-0.2759s^2 - 0.0903s - 0.0084}{s^3 + 3.9507s^2 + 7.6899s + 0.1048} \quad (34)$$

In Figure 5 the reference trajectory and the reacting mixture temperature obtained using H_2/H_∞ controller for the nominal model and for 4 vertex systems are shown. The H_2/H_∞ controller attenuates disturbances fast and the overshoots caused by disturbances are minimal. The trajectory of the controlled variable are almost identical for the

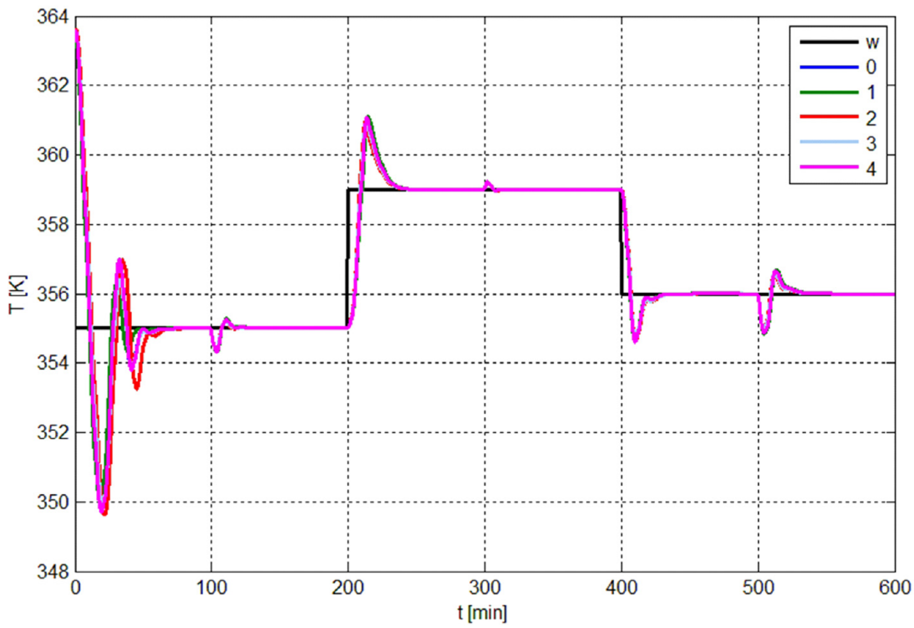

Fig. 3. Small-gain control of the CSTR — the reacting mixture temperature: 0 — nominal system, 1, 2, 3, 4 — vertex systems.

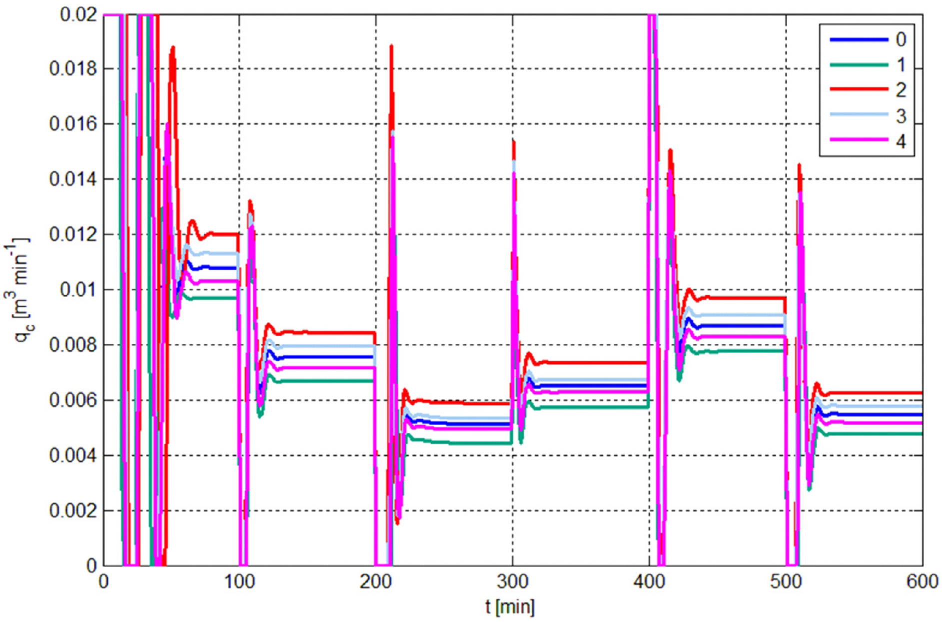

Fig. 4. Small-gain control of the CSTR – the coolant flow rate: 0 – nominal system, 1, 2, 3, 4 – vertex systems.

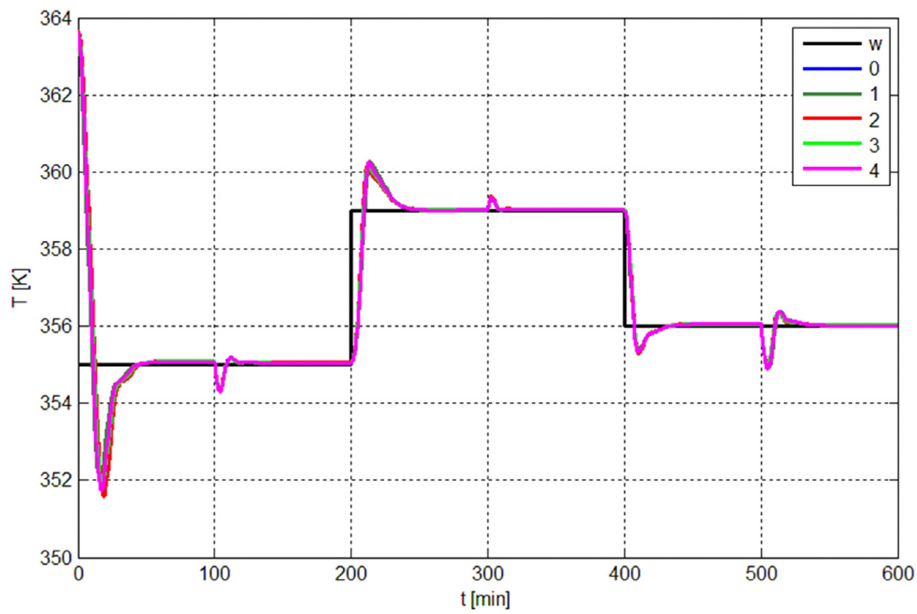

Fig. 5. H_2/H_∞-control of the CSTR – the reacting mixture temperature: 0 – nominal system, 1, 2, 3, 4 – vertex systems.

nominal and all vertex systems. Figure 6 presents the simulation results for the control signal.

The comparison of the proposed controllers was made using *IAE* and *ISE* integral performance indexes described as follows:

$$IAE = \int_0^\infty |e| \mathrm{d}t, \; ISE = \int_0^\infty e^2 \mathrm{d}t \qquad (35)$$

The *IAE* and *ISE* values are given in Table 3. Smaller_*IAE* and *ISE* values were obtained using H_2/H_∞-controller. The lower *IAE* and *ISE* values were achieved by increasing of the *r* value.

Tab. 3. Comparison of the simulation results by *IAE* and *ISE*.

control	small-gain control		H_2/H_∞-controller	
	IAE	*ISE*	*IAE*	*ISE*
nominal system	218	764	186	577
vertex system 1	208	707	178	532
vertex system 2	234	848	199	638
vertex system 3	215	752	190	584
vertex system 4	224	785	186	576

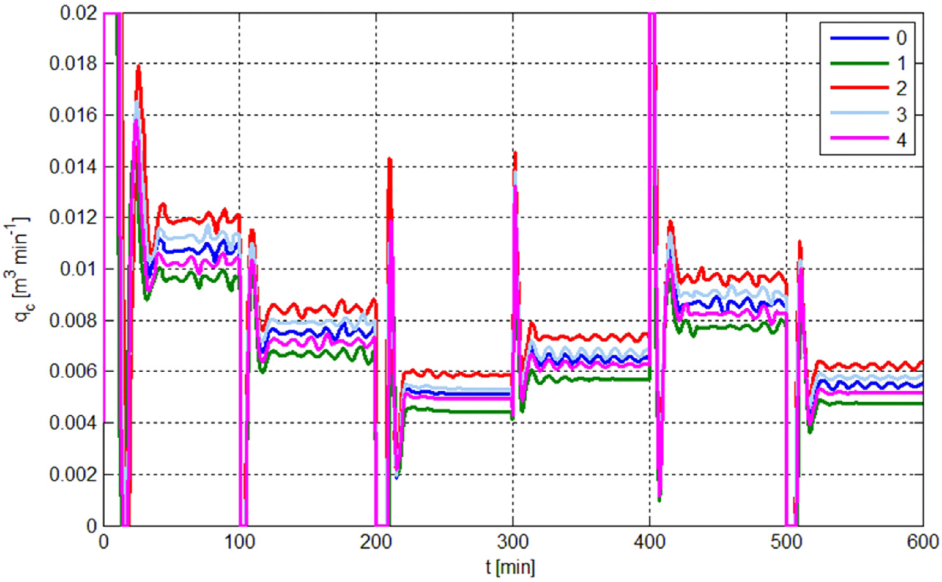

Fig. 6. H_2/H_∞-control of the CSTR – the coolant flow rate: 0 – nominal system, 1, 2, 3, 4 – vertex systems.

Conclusions

The robust controllers have been applied to the control of the exothermic CSTR with uncertain parameters. The controllers were designed using the small gain theorem and the H_2/H_∞ control techniques. Simulations confirmed that designed controllers can be successfully used for control of CSTRs with uncertainties and disturbances, even though the CSTRs are very complicated systems from the control point of view. All simulations were done using MATLAB. Simulation results obtained using designed controllers were compared using integral quality criteria *IAE* and *ISE*. The presented results provide satisfactory control responses for the set-point tracking as well as for the step load disturbance attenuation. The achieved simulation results confirm that the small-gain control and the H_2/H_∞ control are some of the possibilities for successful control of the chemical reactor.

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