Robust PI Control of Chemical Reactors

Jana Závacká, Monika Bakošová, Katarína Vaneková

Institute of Information Engineering, Automation and Mathematics, Faculty of Chemical and Food Technology, STU, Radlinského 9, 812 37 Bratislava, Slovakia

jana.zavacka@stuba.sk

Abstract

The paper presents a method for design of robust PI controllers for systems with interval parametric uncertainty. The proposed method is based on plotting the stability boundary locus in the plane of controller parameters that is called (k_p, k_i)- plane. The designed approach is verified by simulations of control of the continuous stirred tank reactor (CSTR) with hydrolysis of propylene oxide to propylene glycol. The reactor has three uncertain parameters: the reaction enthalpy, the pre-exponential factor in the reaction rate constant and the overall heat transfer coefficient. The control input is the volumetric flow rate of the coolant and the controlled output is the temperature of the reacting mixture.

Keywords: chemical reactor, PI controller, robust control, interval parametric uncertainty

Introduction

Chemical reactors are ones of the most important plants in chemical industry Mikleš and Fikar (2007). Their operation, however, is influenced by many different problems. Some of them arise from varying or not exactly known parameters, as e.g. reaction rate constants or reaction enthalpies. In other cases, reactors have multiple steady-states and their operating points vary. Various types of disturbances also affect operation of chemical reactors. All these problems can cause poor control response or even instability of classical closed-loop control systems. Application of robust control is one way for overcoming all these problems (Alvarez-Ramirez and Femat,1999, Gerhard, 2004, Bakošová et al., 2008, Bakošová et al., 2009).

In this paper, a simple method for design of robust PI controllers is presented (Tan and Kaya 2003). The method is based on plotting the stability boundary locus in the plane of controller parameters that is called (k_p, k_i)-plane. Then, parameters of a stabilizing PI controller are determined from the stability region (Závacká et al.,2009). The PI controller stabilizes a controlled system with interval parametric uncertainty, when the stability region is found for sufficient number of Kharitonov plants (Barmish et al. (1992).

The described approach is used for design of a robust PI controller for a continuous stirred tank reactor with hydrolysis of propylene oxide to propylene glycol that can be modelled in the form of a transfer function with parametric interval uncertainty. The reactor has three uncertain parameters: the reaction enthalpy, the pre-exponential factor in the reaction rate constant and the overall heat transfer coefficient. The control input is the volumetric flow rate of the coolant and the controlled output is the temperature of the reacting mixture. A mathematical model of the reactor has been derived in the form of the 4th order transfer function with interval polynomials in the numerator and the denominator.

Theoretical

Robust PI controller design

Consider a single-input single-output (SISO) control system shown in Fig. 1, where

$$G(s) = \frac{N(s)}{D(s)} \tag{1}$$

is the plant to be controlled and *C(s)* is a PI controller in the form

$$C(s) = \mathrm{k_p} + \frac{k_i}{s} = \frac{k_p s + k_i}{s} \tag{2}$$

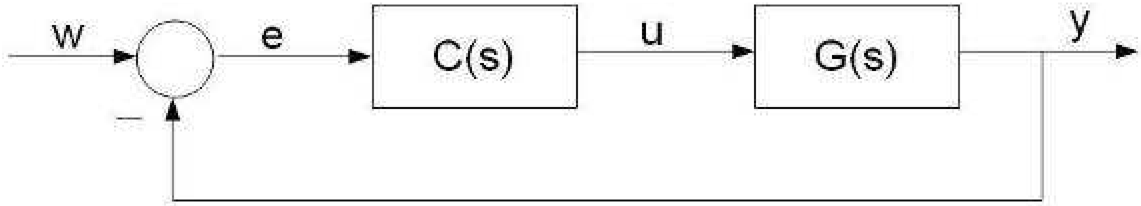

Fig. 1. Control system

The problem is to find the parameters of the PI controller (2) that stabilize the system in Fig. 1, where *w* is the set point, *e* – the control error, *u* – the control input and *y* – the controlled output.

Decomposing the numerator and the denominator polynomials in (1) (Tan and Kaya, 2003) into their even and odd parts, and substituting $s = j\omega$, where ω is the frequency, gives

$$G(j\omega) = \frac{N_e\left(-\omega^2\right) + j\omega N_o\left(-\omega^2\right)}{D_e\left(-\omega^2\right) + j\omega D_o\left(-\omega^2\right)} \tag{3}$$

The closed loop characteristic equation can be written as

$$\begin{aligned} \Delta(j\omega) &= \left[k_i N_e\left(-\omega^2\right) - k_p \omega^2 N_o\left(-\omega^2\right) - \omega^2 D_o\left(-\omega^2\right)\right] + \\ &+ j\left[k_p \omega N_e\left(-\omega^2\right) + k_i \omega N_o\left(-\omega^2\right) + \omega D_e\left(-\omega^2\right)\right] = 0 \end{aligned} \tag{4}$$

Then, equating the real and the imaginary parts of $\Delta(j\omega)$ to zero, one obtains

$$k_p\left(-\omega^2 N_o\left(-\omega^2\right)\right) + k_i\left(N_e\left(-\omega^2\right)\right) = \omega^2 D_o\left(-\omega^2\right) \tag{5}$$

and

$$k_p\left(N_e\left(-\omega^2\right)\right) + k_i\left(N_o\left(-\omega^2\right)\right) = -D_e\left(-\omega^2\right) \tag{6}$$

Let

$$\begin{aligned} F(\omega) &= -\omega^2 N_o\left(-\omega^2\right) \\ G(\omega) &= N_e\left(-\omega^2\right) \\ H(\omega) &= N_e\left(-\omega^2\right) \\ I(\omega) &= N_o\left(-\omega^2\right) \\ J(\omega) &= \omega^2 D_o\left(-\omega^2\right) \\ F(\omega) &= -D_e\left(-\omega^2\right) \end{aligned} \tag{7}$$

Then, (5) and (6) can be written as

$$\begin{aligned} k_p F(\omega) + k_i G(\omega) &= J(\omega) \\ k_p H(\omega) + k_i I(\omega) &= K(\omega) \end{aligned} \tag{8}$$

From (8), parameters of the PI controller (2) are

$$k_p = \frac{J(\omega)I(\omega) - K(\omega)G(\omega)}{F(\omega)I(\omega) - G(\omega)H(\omega)} \tag{9}$$

and

$$k_i = \frac{K(\omega)F(\omega) - J(\omega)H(\omega)}{F(\omega)I(\omega) - G(\omega)H(\omega)} \tag{10}$$

Solving these two equations simultaneously for $\omega \geq 0$, the set of parameters k_p and k_i is obtained. Then, it is possible to plot the dependence of k_i on k_p, and the stability boundary locus $l(k_p, k_i, \omega)$ in the (k_p, k_i)-plane is obtained. The stability boundary divides the parameter plane into stable and unstable regions. The stability region is found by the choice of testing points inside the regions.

The method is very fast and effective, but one problem consists in finding a proper interval of frequency ω. However, the Nyquist plot (Mikleš and Fikar, 2008) can be used for ω rating. It is only necessary to find real values of ω that satisfy condition

$$\mathrm{Im}[G(j\omega)] = 0 . \tag{11}$$

All found stability regions represent values of the PI controller parameters for which the given controlled plant $G(s)$ with interval parametric uncertainty is Hurwitz stable.

Consider a feedback control system (Fig. 1) with the PI controller (2) and the interval plant

$$G(s,b,a) = \frac{N(s,b)}{D(s,a)} = \frac{b_m s^m + b_{m-1} s^{m-1} + \cdots + b_0}{a_n s^n + a_{n-1} s^{n-1} + \cdots + a_0} \tag{12}$$

where $b_i \in [b_i^-, b_i^+]$, $i=0,1,2,\ldots,m,$ and $a_j \in [a_j^-, a_j^+]$, $j=0,1,2,\ldots,n.$ Let the Kharitonov polynomials associated with $N(s,b)$ and $D(s,a)$ are (Barmish, 1994):

$$\begin{aligned} N_1(s) &= b_0^- + b_1^- s + b_2^+ s^2 + b_3^+ s^3 + \ldots \\ N_2(s) &= b_0^+ + b_1^+ s + b_2^- s^2 + b_3^- s^3 + \ldots \\ N_3(s) &= b_0^+ + b_1^- s + b_2^- s^2 + b_3^+ s^3 + \ldots \\ N_4(s) &= b_0^- + b_1^+ s + b_2^+ s^2 + b_3^- s^3 + \ldots \end{aligned} \tag{13}$$

and

$$\begin{aligned} D_1(s) &= a_0^- + a_1^- s + a_2^+ s^2 + a_3^+ s^3 + \ldots \\ D_2(s) &= a_0^+ + a_1^+ s + a_2^- s^2 + a_3^- s^3 + \ldots \\ D_3(s) &= a_0^+ + a_1^- s + a_2^- s^2 + a_3^+ s^3 + \ldots \\ D_4(s) &= a_0^- + a_1^+ s + a_2^+ s^2 + a_3^- s^3 + \ldots \end{aligned} \tag{14}$$

By taking all combinations of the $N_i(s)$ and $D_j(s)$ for i, j = 1,2,3,4, the following family of sixteen Kharitonov plants can be obtained

$$G_K(s) = G_{ij}(s) = \frac{N_i(s)}{D_j(s)}, \qquad i, j = 1, 2, 3, 4; \; K=1, ..., 16 \tag{15}$$

Define the set $S_{ij}(C(s)G_{ij}(s)$ that contains all values of the parameters of the controller $C(s)$ that stabilize $G_{ij}(s)$. Then the set of all the stabilizing parameters of the PI controller that stabilize the interval plant (12), can be written

$$S(C(s)G_K(s)) = S_{11}(C(s)G_{11}(s)) \cap S_{12}(C(s)G_{12}(s)) \cap \cdots \cap S_{44}(C(s)G_{44}(s)). \qquad (16)$$

Experimental

The continuous stirred tank reactor for hydrolysis of propylene oxide to propylene glycol (Molnár et al., 2002, Bakošová et al., 2009), was chosen as a controlled process. The reaction is described as follows

$$C_3H_6O + H_2O \rightarrow C_3H_8O_2 \qquad (17)$$

The reactor is fed with propylene oxide, methanol and water. Methanol is added to improve the solubility of propylene oxide in water. The excess of water provides higher selectivity to propylene glycol and eliminates consecutive reactions of propylene oxide as a key component. Dependence of the reaction rate constant on the reacting mixture temperature is described by the Arrhenius equation

$$k = k_\infty e^{-\frac{E}{RT_r}} \qquad (19)$$

where k_∞ is the pre-exponential factor, E is the activation energy, R is the universal gas constant, and T_r is the temperature of the reacting mixture.

Assuming ideal mixing in the reactor, constant reacting volume, and the same volumetric flow rates of the inlet and outlet streams, the mass balance for any species in the system is

$$V_r \frac{\mathrm{d}c_j}{\mathrm{d}t} = q_r (c_{j0} - c_j) + V_r \nu_j r, \qquad j = 1,2,3 \qquad (20)$$

where V_r is the reacting volume, c_j is the molar concentration of the j-th component, c_{j0} is the feed molar concentration of the j-th component, q_r is the volumetric flow rate of the reacting mixture, v_j is the stoichiometric coefficient of the j-th component, $r = kc_{C_3H_6O}$ is the molar rate of the chemical reaction.

It is assumed further that the specific heat capacities, densities and volumetric flow rates do not depend on temperature or mixture composition, and also the heat of mixing and the mixing volume can be neglected. The simplified enthalpy balance of the reacting mixture used as a standard in reactor design (Ingham et al., 1994) is

$$V_r \rho_r c_{pr} \frac{\mathrm{d}T_r}{\mathrm{d}t} = q_r \rho_r c_{pr} \left(T_{r0} - T_r\right) - UA\left(T_r - T_c\right) + V_r\left(-\Delta_r H\right) r \qquad (21)$$

and the simplified enthalpy balance of the cooling medium is

$$V_c \rho_c c_{pc} \frac{\mathrm{d}T_c}{\mathrm{d}t} = q_c \rho_c c_{pc} \left(T_{c0} - T_r\right) + UA\left(T_r - T_c\right) \qquad (22)$$

where T is the temperature, ρ is the density, c_p is the specific heat capacity, $\Delta_r H$ is the reaction enthalpy, U is the overall heat transfer coefficient, A is the heat exchange area. The subscripts denote: 0 the feed, c the cooling medium, and r the reaction mixture. The values of constant parameters and steady-state inputs of the reactor are summarized in Table 1.

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

parameter	value	steady-state input	value
V_r/m^3	2.407	q_r/(m^3 min^{-1})	0.072
V_c/m^3	2.000	q_c/(m^3 min^{-1})	0.6307
ρ_r/(kg m^{-3})	974.19	T_{rf}/K	299.05
ρ_c/(kg m^{-3})	998	T_{cf}/K	288.15
c_{Pr}/(kJ kg^{-1} K^{-1})	3.7187	c_{f,C_3H_6O} /(kmol m^{-3})	0.0824
c_{Pc}/(kJ kg^{-1} K^{-1})	4.182	$c_{f,C_3H_8O_2}$ /(kmol m^{-3})	0
A/(kJ min^{-1} K^{-1})	8.695		
(E/R)/K	10183		

Model uncertainties of the reactor follow from the fact that there are three physical parameters in this reactor: the reaction enthalpy, the pre-exponential factor and the overall heat transfer coefficient, the values of which vary within certain intervals (Table 2). Nominal values of these parameters are the mean values of the intervals and they are used to derive the reactor nominal model.

Table 2. Uncertain parameters in the CSTR

parameter	minimal	nominal	maximal
$\Delta_r H$/(kJ mol^{-1})	-5.51×10^6	-5.46×10^6	-5.41×10^6
k_∞ /(min^{-1})	2.5867×10^{11}	2.8267×10^{11}	3.0667×10^{11}
U/(kJ min^{-1} m^{-2} K^{-1})	13.0	13.8	14.6

Results and Discussion

For controller design, the mathematical model of the continuous stirred tank reactor with three uncertain parameters (Table 2) is obtained in the form of a transfer function

$$G(s,b,a) = \frac{b_2 s^2 + b_1 s + b_0}{s^4 + a_3 s^3 + a_2 s^2 + a_1 s + a_0} \qquad (23)$$

where coefficients in the numerator polynomial and the denominator one lie in following intervals: $b_2 \in [-0.0297, -0.0240]$, $b_1 \in [-0.0203, -0.0123]$, $b_0 \in [-0.000584, -0.000342]$, $a_3 \in [0.5568, 0.9368]$, $a_2 \in [0.0908, 0.2433]$, $a_1 \in [0.0056, 0.0150]$, $a_0 \in [0.000099, 0.000254]$. Then sixteen Kharitonov plants are created for the reactor and described approach is used for robust PI controller design. The design approach is explained for one of 16 Kharitonov plants. Consider the second Kharitonov plant (i=1, j=2)

$$G_{12}(s) = \frac{-0.0240s^2 - 0.0203s - 0.000584}{s^4 + 0{,}5568s^3 + 0{,}0908s^2 + 0{,}0150s + 0{,}000254} \qquad (24)$$

Equations for calculation of PI controller parameters (9), (10) lead to

$$k_i = \frac{-a_3\omega^4 + a_1\omega^2 + b_1\omega^2\left(\dfrac{-a_4\omega^4 + a_2\omega^2 - a_0}{b_0 - b_2\omega^2}\right)}{-b_2\omega^2 + \dfrac{b_1^2\omega^2}{b_0 - b_2\omega^2} + b_0} \qquad (25)$$

and

$$k_p = \frac{-a_4\omega^4 + a_2\omega^2 - a_0 - b_1 k_i}{b_0 - b_2\omega^2} \qquad (26)$$

Since $\mathrm{Im}[G_{12}(j\omega)] = 0$ is satisfied for $\omega = 0.4123$ rad s^{-1}, it necessary to plot the stability boundary locus for $\omega \in [0, 0.4123]$. The stability region of k_p and k_i is shown in Fig. 2.

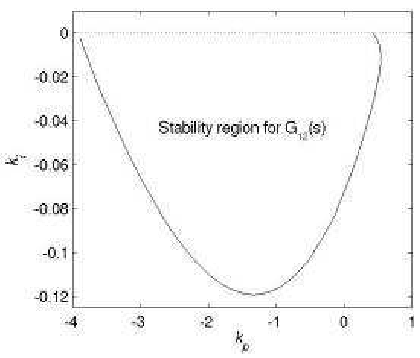

Fig. 2. Stability region for $G_{12}(s)$

The same approach is used to find stability regions for other Kharitonov plants, and the resulting stability region for robust PI controller parameters is found as the intersection of all stability regions. Fig. 3a) shows stability regions found for sixteen Kharitonov plants and Fig. 3b) represents zooming of the intersection of these regions.

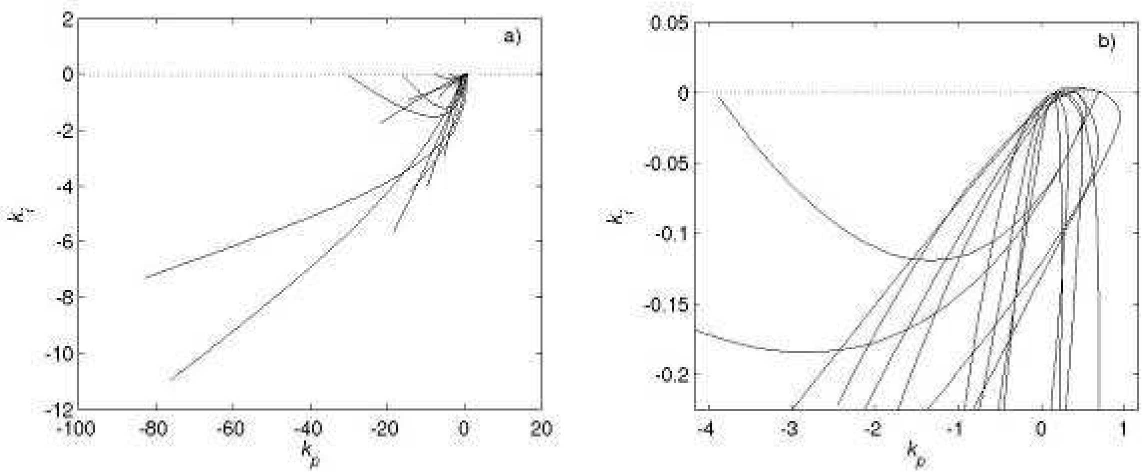

Fig. 3. a) Stability regions for sixteen Kharitonov plants, b) zooming of intersection of stability regions

The parameters k_p and k_i of the PI controller are chosen from the robust stability region shown in Fig. 3b) and the designed PI controller is described by (27)

$$C(s) = \frac{k_p s + k_i}{s} = \frac{-1.2s - 0.03}{s} \tag{27}$$

The robust stability of the closed loop with PI controller (27) is tested using Kharitonov's theorem (Kharitonov (1978). The result of this test is that the closed loop with the interval plant $G(s,b,a)$ (23) and the PI controller $C(s)$ (27) is robustly stable.

The designed robust PI controller (26) is compared with the classical PI controllers tuned by the Stejc method and the Ziegler-Nichols method (Bakošová et al. (2003). The controllers were designed for nominal system (23). The transfer functions of the PI controller tuned by the Strejc method is

$$C_S(s) = Z_R\left(1 + \frac{1}{T_I s}\right) = -0.3688\left(1 + \frac{1}{13.8084s}\right) \tag{28}$$

and the PI controller tuned by the Ziegler-Nichols method is

$$C_{ZN}(s) = Z_R\left(1 + \frac{1}{T_I s}\right) = -1.8520\left(1 + \frac{1}{16.7965s}\right) \tag{29}$$

Integral absolute error (IAE) criterion (Mikleš and Fikar (2007) is one of the most used criteria for judgement of control performance quality and so it is used for comparison of all PI controllers. Obtained results are presented in Table 3 for systems $P_1 – P_8$ and the nominal system P_0. Systems $P_1 – P_8$ represent all nonlinear models of the reactor (20 – 22) that are created for all combinations of boundary values of three uncertain parameters. The nominal system P_0 is the nonlinear model created for mean values of uncertain parameters. These nonlinear models are used as controlled processes in simulation experiments.

Table 3. IAE for designed PI controllers

System	Robust PI controller	Ziegler-Nichols PI controller	Strejc PI controller
P_1	280.3	540.0	420.7
P_2	280.3	540.0	420.7
P_3	204.4	287.8	278.2
P_4	204.4	287.8	278.2
P_5	308.2	566.5	486.1
P_6	308.2	566.5	486.1
P_7	206.0	324.8	296.9
P_8	206.0	324.8	296.9
P_0	232.4	310.4	296.2

It is seen from Table 3 that using the robust PI controller and the PI controller tuned by the Strejc method leads to the smaller IAE then using the PI controller tuned by the Ziegler-Nichols method. Using the Ziegler-Nichols PI controller gives the worst control responses, and so only the control performances obtained using robust and the Strejc PI controllers are presented. Fig. 4 shows control responses obtained for the nominal system P_0. Control responses of systems P_3 with minimal values of IAE are presented in Fig. 5, and Fig. 6 shows control responses obtained for the system P_5 with maximal values of IAE. The control inputs are depicted in Fig. 7.

Both tasks, the setpoint tracking and the disturbance rejection are solved by simulations. The setpoint changes at 0 min from 377.5 K to 381.5 K, at 500 min to 383.5 K and at 1000 min to 379.5 K. The disturbance is generated at 1500 min and is represented by the change of the inlet temperature from 299.0 K to 302.0 K.

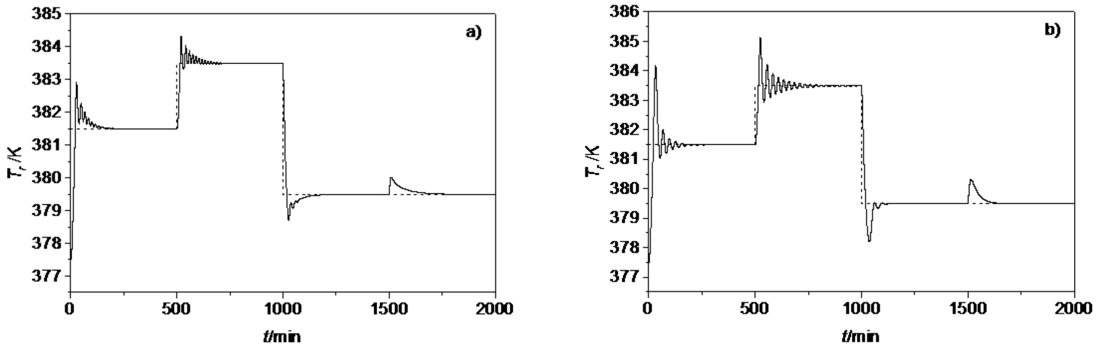

Fig. 4. Control responses of the nominal system P_0 with a) robust PI controller, b) Strejc PI controller: set point (…), controlled output (-)

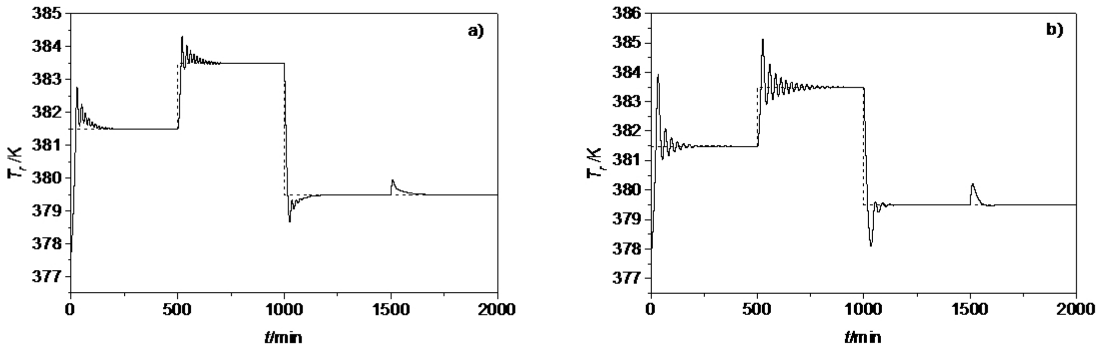

Fig. 5. Control responses of systems with minimal values of IAE obtained using a) robust PI controller, b) Strejc PI controller: set point (…), controlled output (-)

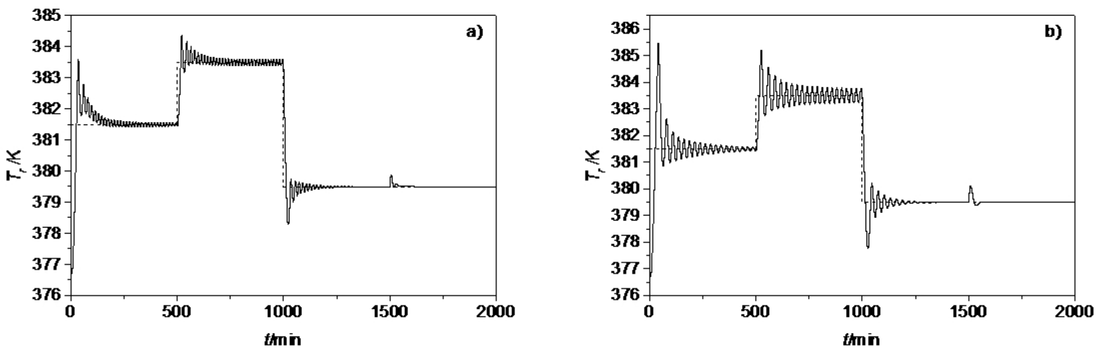

Fig. 6. Control responses of systems with maximal values of IAE obtained using a) robust PI controller, b) Strejc PI controller: set point (…), controlled output (-)

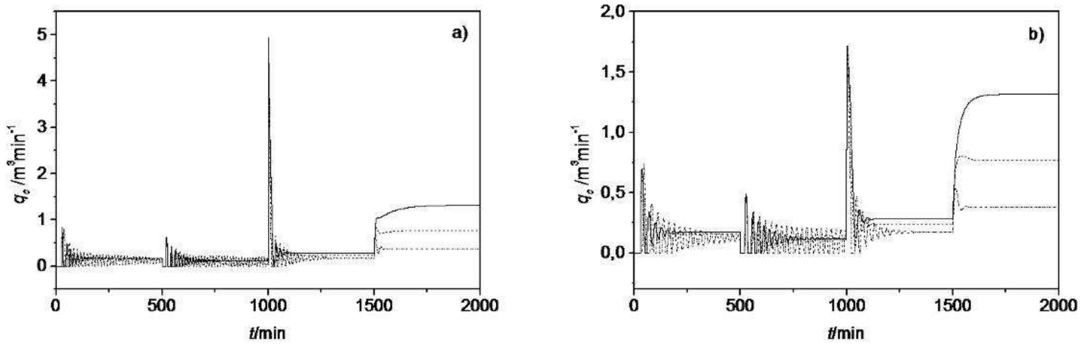

Fig. 7. Control inputs generated by a) robust PI controller, b) Strejc PI controller: nominal system (---), system with minimal IAE (- - -), system with maximal IAE (-.-.-)

Conclusion

In this paper, an approach for design of robust PI controllers is presented. The method is based on finding the stability boundary locus in the plane of controller parameters. The designed robust PI controller is used for simulation of control of an exothermic CSTR with three uncertain parameters. The results obtained by robust PI controller are compared with results obtained by two PI controllers tuned using classical methods: Ziegler-Nichols and Strejc ones. Both, the setpoint tracking and the disturbance rejection are investigated. Presented simulation experiments confirm that all designed PI controllers are able to control the reactor with uncertainties. After comparison of IAE criteria and simulation results, it can be stated that the designed robust PI controller leads to the best results.

Acknowledgement

The authors gratefully acknowledge the contribution of the Scientific Grant Agency of the Slovak Republic under the grants 1/007/09, 1/0537/10 and Development Agency under project APVV-0029-07.

References

Alvarez-Ramirez J, Femat R (1999) Systems Control Letters 38: 219-225

Bakošová M, Fikar M, Čirka Ľ (2003) Základy automatizácie. Laboratórne cvičenia zo základov automatizácie. STU Press, Bratislava

Bakošová M, Puna D, Vasičkaninová A (2008). Acta Chemica Slovaca 1: 12-23

Bakošová M, Puna D, Dostál P, Závacká J (2009) Chemical Papers 63 (5): 527-536

Barmish BR (1994) New tools for robustness of linear systems. MacMillan Publishing Company, New York

Barmish BR, Hollt CV, Kraus FJ, Tempo R (1992) IEEE Transactions on Automatic Control, AC-37, 707-714

Gerhard J, Mönningmann M, Marquardt W (2004) Proceedings of the "7th International Symposium on Dynamics and Control of Process Systems", Massachusetts, July 5 – 7, 2004, 92 p.

Ingham J, Dunn IJ, Heinzle E, Přenosil JE (1994) Chemical Engineering Dynamics. VCH Verlagsgesellschaft , Weinheim.

Kharitonov VL (1978) Differential Equations 14: 1483-1485.

Mikleš J, Fikar M (2007) Process Modelling, Identification, and Control. Springer Verlag, Berlin Heidelberg

Molnár A, Markoš J, Jelemenský Ľ (2002) Chemical Papers 56: 357-361

Tan N, Kaya I (2003) Mediterranean Conference on Control and Automation, Rhodes, Greece

Závacká J, Bakošová M, Vaneková K (2009) Automatizace 52 (6): 362-365