

Robust Control of Chemical Reactors

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Abstract

The possibility to use robust PI controllers for stabilization of continuous stirred tank reactors is discussed in this paper. Considered reactors are exothermic ones with multiple steady states and uncertain parameters. A computationally simple non-iterative algorithm is used for the robust static output feedback PI controller design. The design procedure guarantees with sufficient conditions the robust quadratic stability and the guaranteed cost. Designed robust PI controllers are able to stabilize the reactors with uncertainty in their unstable steady states.

Keywords: chemical reactor, PI controller, robust control, static output feedback

Introduction

Chemical reactors are ones of the most important plants in chemical industry. Their operation, however, is connected with 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, see e.g. Alvarez-Ramirez and Fermat (1999), Gerhard (2004), Bakošová et al. (2005).

Robust control has grown as one of the most important areas in modern control design since works by Doyle (1981), Zames (1983) and many others. One of the solved problems is also the problem of robust static output feedback control (RSOFC), which has been till now an important open question in control engineering, see e.g. Iwasaki (1994), Syrmos (1997) and references therein. Various approaches have been used to study two aspects of the robust stabilization problem.

The first aspect is related to conditions under which the linear system described in the state space can be stabilized via output feedback. The necessary and sufficient conditions for stabilization of a linear continuous-time invariant system via static output feedback can be found e.g. in Kučera (1995) and for stabilization of an uncertain affine linear systems e.g. in Veselý (2004). Recently, it has been shown that an extremely wide array of robust controller design problems can be reduced to the linear matrix inequalities (LMIs) problem. Specially, the LMIs in semi-definite programming attract a big interest because of their ability to describe non-trivial control design problems integrating various specifications such as robustness, structural and performance constraints, as well as their suitability for efficient numerical processing through various available solvers, see e.g. Boyd (1994) and references therein.

The second aspect of the robust stabilization problem is related to a procedure for obtaining a stabilizing or robustly stabilizing control law. Most of recent works present iterative algorithms in which sets of LMI problems are repeated until certain convergence criteria are met, see e.g. Cao and Sun (1998), Bernussou (2005).

Necessary and sufficient conditions for stabilization of an uncertain polytopic system using static output feedback are formulated in this paper at first. The polytopic uncertainty is considered, while it is recognized as one of the most difficult structured uncertainties. Then the problem of robust controller design is transformed to the LMI problems. A computationally simple LMI based non-iterative algorithm is used for the design of robust static output feedback controllers. The design procedure assures with sufficient conditions the quadratic stability of the closed-loop system and the guaranteed cost of control. Designed robust PI controllers are used for stabilization of a continuous-time stirred tank reactor (CSTR) with two uncertain parameters in its unstable steady state.

Theoretical

The robust static output feedback controller design is based on a state-space representation of a controlled process. Consider the controlled process is an uncertain linear time variant system in the form

$$\begin{aligned}\dot{\mathbf{x}}(t) &= \mathbf{A}(t)\mathbf{x}(t) + \mathbf{B}(t)\mathbf{u}(t), & \mathbf{x}(t_0) &= \mathbf{x}_0 \\ \mathbf{y}(t) &= \mathbf{C}(t)\mathbf{x}(t)\end{aligned}\tag{1}$$

where t is time, $\mathbf{x}(t)$ is the n -dimensional vector of state variables, $\mathbf{u}(t)$ is the m -dimensional vector of control variables, $\mathbf{y}(t)$ is the l -dimensional vector of output variables, the subscript 0

represents the origin and matrices $A(t)$, $B(t)$, $C(t)$ have appropriate dimensions. Consider further that under the assumption of slowly varying parameters, the system represented by (1) is a polytop of linear time invariant systems

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \mathbf{A}_i \mathbf{x}(t) + \mathbf{B}_i \mathbf{u}(t), \quad \mathbf{x}(t_0) = \mathbf{x}_0 \\ \mathbf{y}(t) &= \mathbf{C}_i \mathbf{x}(t) \\ i &= 1, \dots, N \end{aligned} \quad (2)$$

which represent vertices of (1). The number of vertex systems $N = 2^p$, where p is the number of uncertain parameters of (1).

The problem of robust static output feedback control design can be formulated as follows. For the system (1) find a proportion of the output signal $\mathbf{y}(t)$, which is passed (fed back) to the control input $\mathbf{u}(t)$ according to (3)

$$\mathbf{u}(t) = \mathbf{F}\mathbf{y}(t) \quad (3)$$

The matrix \mathbf{F} represents the static output feedback controller and the closed-loop system using (3) is described as follows

$$\dot{\mathbf{x}}(t) = [\mathbf{A}(t) + \mathbf{B}(t)\mathbf{F}\mathbf{C}(t)]\mathbf{x}(t) = \mathbf{A}_{CL}(t)\mathbf{x}(t) \quad (4)$$

where $\mathbf{A}_{CL}(t)$ is the state matrix of the closed-loop system and it is a convex envelope of a set of linear time invariant matrices \mathbf{A}_{CLi}

$$\mathbf{A}_{CLi} = \mathbf{A}_i + \mathbf{B}_i\mathbf{F}\mathbf{C}_i, \quad i = 1, \dots, N \quad (5)$$

which represent state matrices of the closed-loop vertex systems.

Design of \mathbf{F} is very important when the system (1) is unstable. In this case, it is necessary to find the static output feedback (3) such that the closed-loop system (4) is stable. The design procedure for \mathbf{F} is based on formulation of necessary and sufficient conditions for quadratic stability of (1), simultaneous quadratic stabilizability of (1) and quadratic stabilizability of (1) with guaranteed cost.

The system (1) is quadratically stable if and only if there exists a positive definite matrix $\mathbf{P} > 0$ such that the following inequalities are satisfied (Vesely 2002)

$$\mathbf{A}_i^T \mathbf{P} + \mathbf{P} \mathbf{A}_i < 0, \quad \mathbf{P} > 0, \quad i = 1, \dots, N \quad (6)$$

Consequently, the system (1) is simultaneously static output feedback quadratically stabilizable, e. a. all vertices (2) of (1) are static output feedback quadratically stabilizable, if and only if there exist a positive definite matrix $\mathbf{P} > 0$ and a feedback matrix \mathbf{F} such that following inequalities are satisfied (Vesely 2002)

$$\mathbf{A}_{CLi}^T \mathbf{P} + \mathbf{P} \mathbf{A}_{CLi} < 0, \quad \mathbf{P} > 0, \quad i = 1, \dots, N \quad (7)$$

Consider further, that it is necessary to stabilize the system (1) with guaranteed cost J^*

$$\int_0^{\infty} [\mathbf{x}(t)^T \mathbf{Q} \mathbf{x}(t) + \mathbf{u}(t)^T \mathbf{R} \mathbf{u}(t)] dt \leq \mathbf{x}_0^T \mathbf{P} \mathbf{x}_0 = J^*, \mathbf{P} > 0 \quad (8)$$

where \mathbf{Q} and \mathbf{R} are weighting matrices. The system (1) is simultaneously output feedback stabilizable with guaranteed cost J^* if there exist matrices $\mathbf{P} > 0$, $\mathbf{Q} > 0$, $\mathbf{R} > 0$ and a matrix \mathbf{F} such that the following inequalities hold (Veselý 2002)

$$\mathbf{A}_i^T \mathbf{P} + \mathbf{P} \mathbf{A}_i - \mathbf{P} \mathbf{B}_i \mathbf{R}^{-1} \mathbf{B}_i^T \mathbf{P} + \mathbf{Q} \leq 0, \quad i = 1, \dots, N \quad (9)$$

$$\left(\mathbf{B}_i^T \mathbf{P} + \mathbf{R} \mathbf{F} \mathbf{C}_i \right) \Phi_i^{-1} \left(\mathbf{B}_i^T \mathbf{P} + \mathbf{R} \mathbf{F} \mathbf{C}_i \right)^T - \mathbf{R} \leq 0, \quad i = 1, \dots, N \quad (10)$$

where

$$\Phi_i = - \left(\mathbf{A}_i^T \mathbf{P} + \mathbf{P} \mathbf{A}_i - \mathbf{P} \mathbf{B}_i \mathbf{R}^{-1} \mathbf{B}_i^T \mathbf{P} + \mathbf{Q} \right), \quad i = 1, \dots, N \quad (11)$$

Design procedure

The design procedure for simultaneous static output feedback stabilization of the system (1) with guaranteed cost (8) is based on the statements formulated above and their transformation to LMIs. Using Schur complement formula (Boyd et al. 1994) and defining $\mathbf{S} = \mathbf{P}^{-1}$, the inequalities (9) are transformed to the following LMIs

$$\begin{bmatrix} \mathbf{S} \mathbf{A}_i^T + \mathbf{A}_i \mathbf{S} - \mathbf{B}_i \mathbf{R}^{-1} \mathbf{B}_i^T & \mathbf{S} \sqrt{\mathbf{Q}} \\ \sqrt{\mathbf{Q}} \mathbf{S} & -\mathbf{I} \end{bmatrix} < 0, \quad \gamma \mathbf{I} < \mathbf{S}, \quad i = 1, \dots, N \quad (12)$$

where $\gamma > 0$ is any non-negative constant.

Similarly, the inequalities (10) are transformed to the following LMIs

$$\begin{bmatrix} -\mathbf{R} & \mathbf{B}_i^T \mathbf{P} + \mathbf{R} \mathbf{F} \mathbf{C}_i \\ \left(\mathbf{B}_i^T \mathbf{P} + \mathbf{R} \mathbf{F} \mathbf{C}_i \right)^T & -\Phi_i \end{bmatrix} < 0, \quad i = 1, \dots, N \quad (13)$$

The algorithm for finding a robust static feedback controller, which assures simultaneous stabilization of the system (1) with guaranteed cost J^* (8), is following.

1. Compute $\mathbf{S} = \mathbf{S}^T > 0$ from the LMIs (12).
2. $\mathbf{P} = \mathbf{S}^{-1}$.
3. Compute \mathbf{F} from the LMIs (13).
4. If the solution of (12) is not feasible, the system (1) is not simultaneously stabilizable using static output feedback. If the solution of (13) is not feasible, the closed-loop system (1) is not quadratically stable with guaranteed cost. Then it is necessary to change \mathbf{Q} , \mathbf{R} in (8) or γ in (12) in order to find feasible solutions. If the solutions of (12) and (13) are feasible, then the

system (1) is simultaneously stabilizable and the system (1) is quadratically stable with guaranteed cost J^* (8).

Experimental

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. 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 other usual simplifications (Ingham et al. 1994), the model of the CSTR can be described by four nonlinear differential equations

$$\frac{dc_A}{dt} = -\left(\frac{q_r}{V_r} + k_1 + k_2\right)c_A + \frac{q_r}{V_r}c_{Af} \quad (14)$$

$$\frac{dc_B}{dt} = -\frac{q_r}{V_r}c_B + k_1c_A + \frac{q_r}{V_r}c_{Bf} \quad (15)$$

$$\frac{dT_r}{dt} = -\frac{(\Delta_r H)_1 k_1 + (\Delta_r H)_2 k_2}{\rho_r c_{Pr}}c_A + \frac{q_r}{V_r}(T_{rf} - T_r) + \frac{A_h U}{V_r \rho_r c_{Pr}}(T_c - T_r) \quad (16)$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c}(T_{cf} - T_c) + \frac{A_h U}{V_c \rho_c c_{Pc}}(T_r - T_c) \quad (17)$$

with initial conditions $c_A(0)$, $c_B(0)$, $T_r(0)$ and $T_c(0)$. Here, t is time, c is the concentration, T is the temperature, V is the volume, ρ is the density, c_p is the mass heat capacity, q is the volumetric flow rate, $(\Delta_r H)$ is the reaction enthalpy, A_h is the heat exchange area and U is the overall heat exchange coefficient. The subscripts denote: r – the reacting mixture, c – the coolant, f – the feed value and the superscript s denotes the steady-state value. The reaction rates k_1 , k_2 are described by Arrhenius equations

$$k_j = k_{\infty j} \exp\left(-\frac{E_j}{RT_r}\right), j = 1, 2 \quad (18)$$

where k_{∞} is the pre-exponential factor, E is the activation energy and R is the universal gas constant.

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 only approximately known physical parameters in this reactor: pre-

exponential factors in the reaction rate constants (18). Their values are presented in Table 2. The nominal values of these parameters are mean values of their intervals.

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

Parameter	Value	Steady-state input	Value
V_r/m^3	0.23	$q_r/(\text{m}^3 \text{min}^{-1})$	0.015
V_c/m^3	0.21	$q_c/(\text{m}^3 \text{min}^{-1})$	0.004
$\rho_r/(\text{kg m}^{-3})$	1020	T_{rf}/K	310
$\rho_c/(\text{kg m}^{-3})$	998	T_{cf}/K	288
$c_{Pr}/(\text{kJ kg}^{-1} \text{K}^{-1})$	4.02	$c_{Af}/(\text{kmol m}^{-3})$	4.22
$c_{Pc}/(\text{kJ kg}^{-1} \text{K}^{-1})$	4.182	$c_{Bf}/(\text{mol m}^{-3})$	0
$A_h U/(\text{kJ min}^{-1} \text{K}^{-1})$	64.628		
$(E_1/R)/\text{K}$	9850		
$(E_2/R)/\text{K}$	22019		
$(\Delta_r H)_1/(\text{kJ kmol}^{-1})$	-8.6×10^4		
$(\Delta_r H)_2/(\text{kJ kmol}^{-1})$	-5.5×10^4		

Table 2. Uncertain parameters in the CSTR

parameter	minimal	nominal	maximal
$k_{1\infty} / \text{min}^{-1}$	1.5×10^{11}	1.55×10^{11}	1.6×10^{11}
$k_{2\infty} / \text{min}^{-1}$	5.95×10^{26}	8.55×10^{26}	11.15×10^{26}

It is supposed for control purposes that the reactor is a two-input two-output system. The reacting mixture flow rate q_r and the coolant flow rate q_c are chosen as the control inputs and the temperature of the reacting mixture T_r and the temperature of the coolant T_c are chosen as the controlled outputs. The other input variables are considered to be constant.

Steady-state and open-loop analysis

The steady-state behaviour of the chemical reactor was studied at first. The results of the steady-state analysis of the CSTR with nominal values of uncertain parameters are shown in Fig. 1, where the curve Q_{GEN} is the heat generated by chemical reactions and the line Q_{OUT}

is the heat removed by the jacket and the product stream. The steady-state temperatures of the reacting mixture were determined from intersections of Q_{GEN} and Q_{OUT} . The results obtained for all four combinations of minimal and maximal values of uncertain parameters were similar. It can be stated the reactor has always three steady states, two of them are stable and one is unstable. The maximal concentration of the main product B is obtained in the unstable steady state of the CSTR, as it is seen in Fig. 2 for the nominal model. So, it can be important to stabilize the CSTR in its unstable steady state characterized by the temperatures of the reacting mixture $T_r^s = 338.4$ K and the coolant $T_c^s = 328.1$ K.

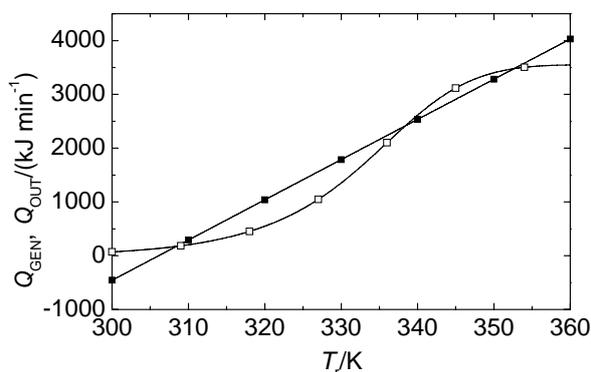


Fig. 1. Three steady states of the CSTR: Q_{GEN} (\square), Q_{OUT} (\bullet)

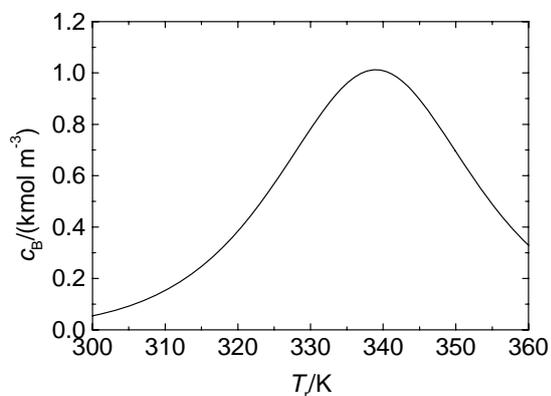


Fig. 2. Concentration of the main product B in the dependence on the T_r

In this context, the open-loop behaviour of the reactor in the surroundings of its unstable steady state was also studied. The initial temperatures of the reaction mixture and the coolant were chosen $T_r(0) = 341.3$ K and $T_c(0) = 330.3$ K. Simulation results obtained for the nominal model and also for 4 vertex systems are shown in Fig. 3. They confirm that without feedback control, the CSTR cannot be stabilized in its unstable steady state and the

temperature of the reaction mixture in the CSTR and the temperature of the coolant in the jacket converge to one of two stable steady states.

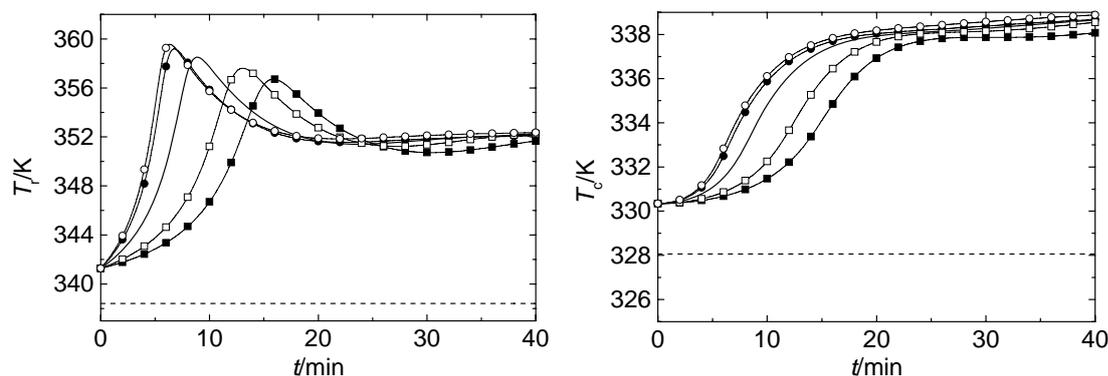


Fig. 3. Open-loop response of the CSTR: main operating point (---), nominal system (—), vertex systems (—□—, —●—, —□—, —○—)

Results and Discussion

It is clear from the steady-state and open-loop analysis that it is necessary to stabilize the reactor in its unstable steady state (main operating point) using suitable feedback control for maximal production of the main product B. The robust control approach was chosen for the controller design because of presence of uncertainty in the reactor kinetics. The design of robust stabilizing PI controllers was based on the theory presented in the theoretical section.

The linear state space model (1) of the CSTR was derived using linearization of non-linear terms in material and enthalpy balances (14) – (17). For the sake of adding an integral part to the controller, it was necessary to augment matrices of the linear state space description of the CSTR (Mikleš 2006). The matrices of the nominal linear model in the main operating point with respect to the integral part of the controller are

$$\mathbf{A}_0 = \begin{pmatrix} -0.1479 & 0 & -0.0226 & 0 & 0 & 0 \\ 0.0354 & -0.0652 & 0.0057 & 0 & 0 & 0 \\ 1.3763 & 0 & 0.2118 & 0.0685 & 0 & 0 \\ 0 & 0 & 0.0737 & -0.0928 & 0 & 0 \\ 0 & 0 & 1.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0 & 0 & 0 \end{pmatrix}, \mathbf{B}_0 = \begin{pmatrix} 10.2546 & 0 \\ -4.3968 & 0 \\ -123.5131 & 0 \\ 0 & -190.7612 \\ 0 & 0 \\ 0 & 0 \end{pmatrix},$$

$$\mathbf{C}_0 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

For 2 uncertain parameters, we obtained $2^2 = 4$ linear models, which represent vertices of the uncertain polytopic system (2). Nominal system and all vertex systems are unstable. The design procedure described in the previous section was used for finding a stabilizing output feedback PI controller. There are three parameters, which influence solution and can be changed: \mathbf{Q} , \mathbf{R} and γ . In dependence on the choice of these parameters, it was possible to find several stabilizing controllers, which stabilized the polytopic system with 4 vertices. Some of them are presented in Table 3. Guaranteed costs are also included. For all stabilizing PI controllers \mathbf{F} , the closed loop systems obtained for the nominal system and also for 4 vertex systems are stable.

The designed robust PI controllers were tested by simulations on the nonlinear mathematical model of the CSTR. The initial temperatures of the reaction mixture and the coolant were again $T_r(0) = 341.3$ K and $T_c(0) = 330.3$ K. The goal was to bring the CSTR to the main operating point given by the temperatures of the reaction mixture $T_r^s = 338.4$ K and the coolant $T_c^s = 328.1$ K. The simulation results obtained with the robust static output feedback controller $\mathbf{F} = \begin{pmatrix} 0.0239 & 0.0016 & 0.0013 & 0.0001 \\ 0.0379 & 0.1363 & 0.0032 & 0.0046 \end{pmatrix}$ are shown in Figs. 4, 5. It can be stated the designed robust PI controller is stable to stabilize the CSTR in its unstable steady state.

Table 3. Robust stabilizing controllers for the CSTR

\mathbf{Q}	\mathbf{R}	γ	\mathbf{F}^T	J^*
diag(0.1,0.1,0.01,0.01, 0.001,0.001)	$\begin{pmatrix} 50 & 0 \\ 0 & 100 \end{pmatrix}$	0.001	$\begin{pmatrix} 0.0997 & 0.0044 \\ 0.0019 & 0.1104 \\ 0.0674 & 0.0034 \\ 0.0012 & 0.0828 \end{pmatrix}$	10.9983
diag(0.1,0.1,0.001,0.001, 0.00001,0.00001)	$\begin{pmatrix} 0.01 & 0 \\ 0 & 0.01 \end{pmatrix}$	0.001	$\begin{pmatrix} 0.0239 & 0.0379 \\ 0.0016 & 0.1363 \\ 0.0013 & 0.0032 \\ 0.0001 & 0.0046 \end{pmatrix}$	1.5070
diag(0.1,0.1,0.01,0.01, 0.0001,0.0001)	$\begin{pmatrix} 0.01 & 0 \\ 0 & 0.01 \end{pmatrix}$	1	$\begin{pmatrix} 0.0499 & 0.0010 \\ -0.0264 & 0.5260 \\ 0.0114 & -0.0184 \\ -0.0096 & 0.1594 \end{pmatrix}$	0.0003

The ability of the robust PI controller to stabilize the CSTR in the presence of disturbances was also studied. Occurrence of a disturbance in the feed temperature of the reaction mixture was supposed. T_{rf} increased by 5 K for $t \geq 40$ min. The obtained simulation results are shown in Figs. 6, 7. It is clear from these simulation experiments that the robust static output feedback controller is able to stabilize the CSTR with uncertainties in its unstable steady state also in the presence of a disturbance.

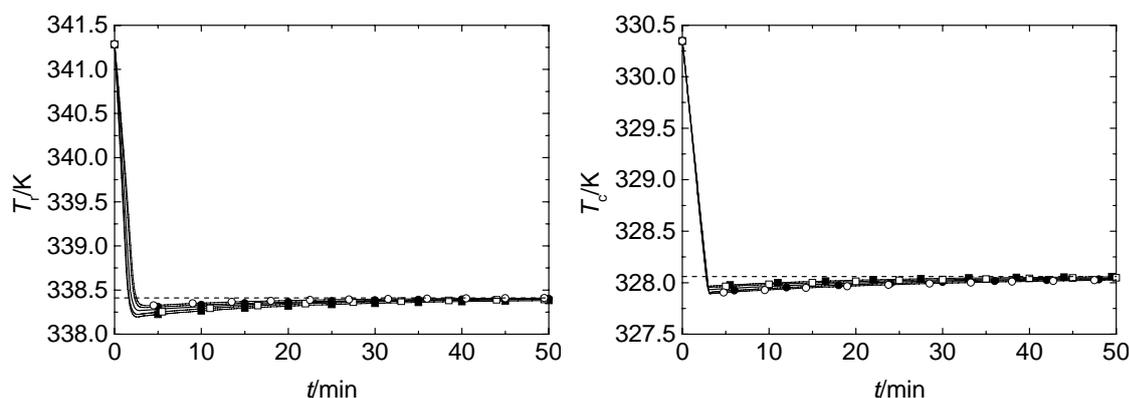


Fig. 4. Robust control of the CSTR: main operating point (---), nominal system (—), vertex systems (—□—, —●—, —□—, —○—)

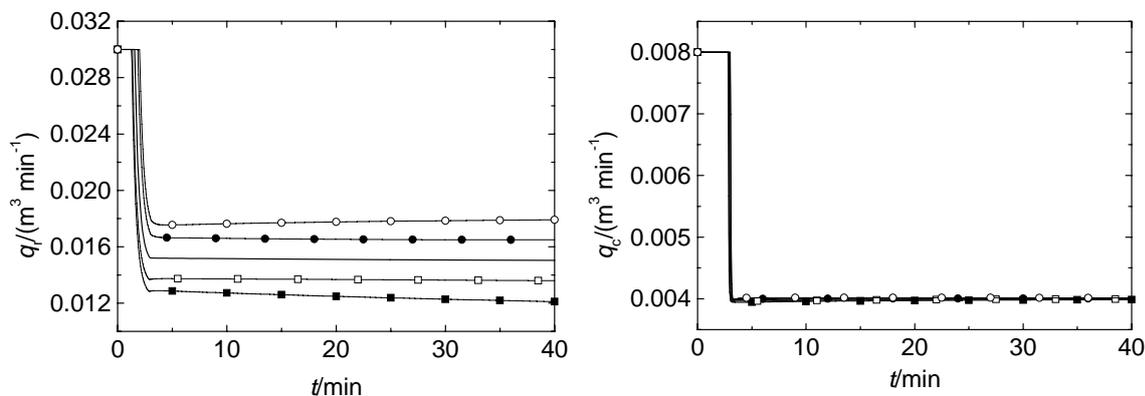


Fig. 5. Control inputs to the CSTR: nominal system (—), vertex systems (—□—, —●—, —□—, —○—)

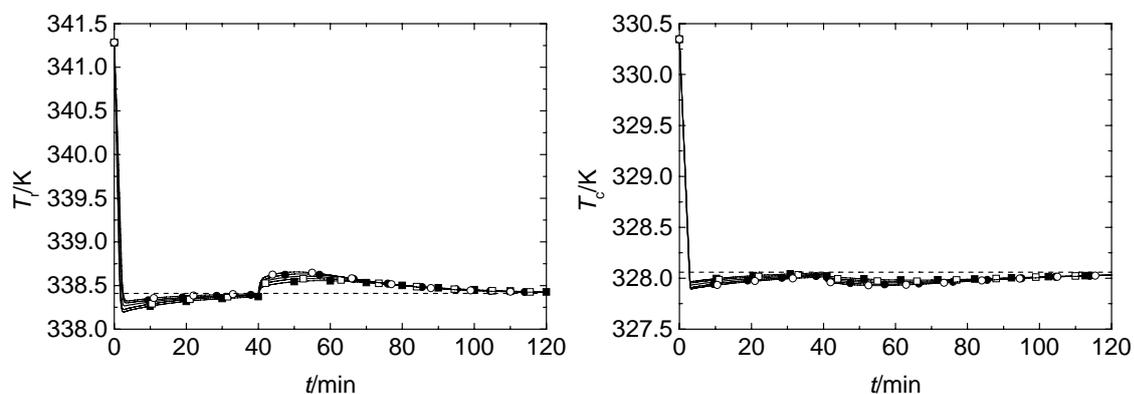


Fig. 6. Robust control of the CSTR in the presence of a disturbance: main operating point (---), nominal system (—), vertex systems (—□—, —●—, —○—)

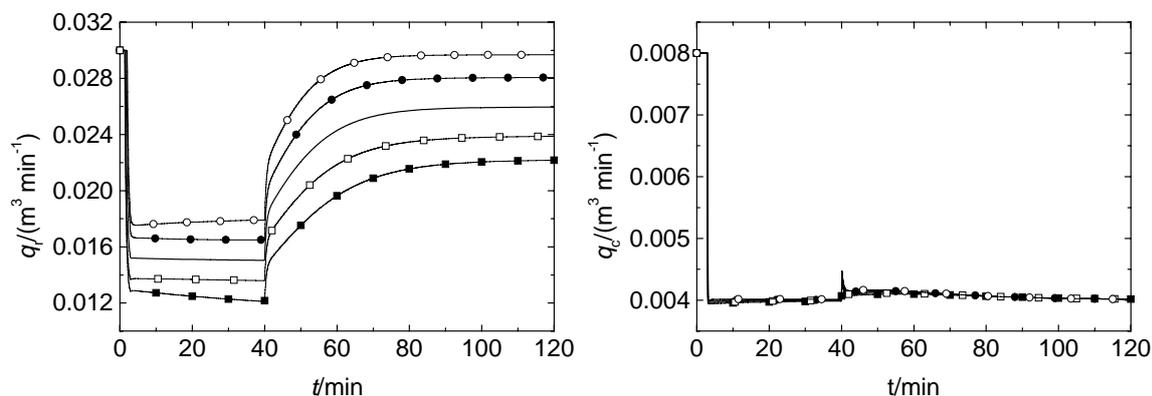


Fig. 7. Control inputs to the CSTR in the presence of a disturbance: nominal system (—), vertex systems (—□—, —●—, —○—)

Conclusion

The possibility to stabilize the exothermic chemical reactor with two uncertain parameters using robust static output feedback PI controllers is studied in this paper. The results confirm that the presented simple non-iterative algorithm based on solving of two sets of LMIs is an effective tool for the design of robust stabilizing controllers. Such robust controllers can be successfully used for control of CSTRs with multiple steady states, uncertainties and disturbances, even though the CSTRs are very complicated systems from the control viewpoint. The disadvantage of the presented design is the necessity to choose the parameters \mathbf{Q} , \mathbf{R} and γ . The coefficients of \mathbf{Q} and \mathbf{R} can be chosen with respect to physical values of state and input variables, but the ad-lib choice gives sometimes better controllers. The advantage of the robust controller design consists in the fact that robust controllers are designed off-line and there is a possibility to test their properties e.g. by simulations before practical using. The advantage of using of robust PI controllers is that they do not retain offsets.

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