Robust stabilization of an exothermic CSTR
Proceedings of European Congress of Chemical Engineering (ECCE-6)
Copenhagen, 16-20 September 2007

Robust stabilization of an exothermic CSTR

M. Bakošová, D. Puna, J. Závacká

Department of Information Engineering and Process Control, Institute of Information Engineering, Automation and Mathematics, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovakia

Abstract

The paper deals with an application of robust static output feedback control to an exothermic continuous-time stirred tank reactor with parametric uncertainties and multiple steady states. The problem of robust controller design is converted to solution of linear matrix inequalities and a computationally simple non-iterative algorithm is presented. The possibility to use robust static output feedback for stabilization of reactors with uncertainties and comparison of a robust controller with an optimal controller is demonstrated by simulation results.

Keywords: chemical reactor, multiple steady states, uncertainty, robust control, static output feedback

1. Introduction

Exothermic reactors are very interesting systems because of their potential safety problems and the possibility of exotic behavior such as multiple steady states (Molnár, A. et al., 2002). Furthermore, operation of chemical reactors is corrupted by many different uncertainties. Some of them arise from varying or not exactly known parameters, as e.g. chemical kinetics or reaction activity. In other cases operating points change. Various types of perturbations also affect chemical reactors. All these uncertainties can cause poor performance or even instability of closed-loop control systems (Kuník et al., 2006). Application of robust control approach can be one way to overcome all these problems as it is shown e.g. in Gerhard et al. (2004), Bakošová et. al. (2005) and others.

Robust control has grown as one of the most important areas in modern control design since works by Zames (1981), Doyle (1981) and many others. One of the up to now opened problems is also the problem of a robust static output feedback (Syrmos et al., 1997). 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 can be found e.g. in Kučera and de Souza (1995), Veselý (2004). The second aspect is related to finding a procedure for obtaining a stabilizing or robustly stabilizing control law. It has been shown that an extremely wide array of robust controller design problems can be reduced to the problem of finding feasible solutions of LMIs (Boyd et al., 1994). LMIs have been used to design of robust output feedback controllers e.g. in Benton and Smith (1999), Henrion et al. (1999), Veselý (2002) and others.

The goal of this paper is to present the possibility to stabilize a continuous stirred tank reactor (CSTR) with an exothermic reaction (hydrolysis of propylene oxide to propylene glycol) in its unstable steady state using robust static output feedback control (RSOFC). The CSTR is an uncertain system because of two inexactly known physical parameters, reaction rate constant and heat of reaction. A computationally simple LMI based non-iterative algorithm is used for design of robust static output feedback controller (Veselý, 2002). The designed robust controller is used to stabilization of the exothermic CSTR with uncertainties.

The paper is organized as follows. In section 2, basic principles of RSOFC are summarized. The CSTR is described in section 3, and simulation results are presented in section 4. Finally, in section 5 main conclusions are drawn.

2. Robust static output feedback control

2.1. Robust static output feedback, robust quadratic stability and guaranteed cost

Consider an uncertain linear time variant system S in the form

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

with

$$\boldsymbol{A}(t) \in \mathrm{Co}\{\boldsymbol{A}_1,\ldots,\boldsymbol{A}_N\} := \left\{ \sum_{i=1}^{N} \alpha_i \boldsymbol{A}_i : \alpha_i \geq 0, \sum_{i=1}^{N} \alpha_i = 1 \right\} \tag{2}$$

$$\boldsymbol{B}(t) \in \mathrm{Co}\{\boldsymbol{B}_1,\ldots,\boldsymbol{B}_N\} := \left\{ \sum_{i=1}^{N} \alpha_i \boldsymbol{B}_i : \alpha_i \geq 0, \sum_{i=1}^{N} \alpha_i = 1 \right\} \tag{3}$$

$$\boldsymbol{C}(t) \in \mathrm{Co}\{\boldsymbol{C}_1,\ldots,\boldsymbol{C}_N\} := \left\{ \sum_{i=1}^{N} \alpha_i \boldsymbol{C}_i : \alpha_i \geq 0, \sum_{i=1}^{N} \alpha_i = 1 \right\} \tag{4}$$

where $x(t) \in R^n$ is the state, $u(t) \in R^m$ the control and $y(t) \in R^r$ the output. $\mathrm{Co}\{\boldsymbol{A}_1,\ldots,\boldsymbol{A}_N\}$, $\mathrm{Co}\{\boldsymbol{B}_1,\ldots,\boldsymbol{B}_N\}$ and $\mathrm{Co}\{\boldsymbol{C}_1,\ldots,\boldsymbol{C}_N\}$ are convex envelopes of sets of linear time invariant (LTI) matrices $\boldsymbol{A}_i$, $\boldsymbol{B}_i$, $\boldsymbol{C}_i$, $i = 1,\ldots,N,$ and matrices $\boldsymbol{A}_i$, $\boldsymbol{B}_i$, $\boldsymbol{C}_i$ have appropriate dimensions. The system represented by (1) is a polytop of linear time invariant systems S_i, $i=1,\ldots,N$,

$$\dot{\boldsymbol{x}}(t)=\boldsymbol{A}_i\boldsymbol{x}(t)+\boldsymbol{B}_i\boldsymbol{u}(t),\quad \boldsymbol{x}(t_0)=\boldsymbol{x}_0$$
$$\boldsymbol{y}(t)=\boldsymbol{C}_i\boldsymbol{x}(t) \tag{5}$$

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

Consider also an uncertain polytopic closed-loop system

$$\dot{\boldsymbol{x}}(t)=\left[\boldsymbol{A}(t)+\boldsymbol{B}(t)\boldsymbol{F}\boldsymbol{C}(t)\right]\boldsymbol{x}(t)=\boldsymbol{A}_{CL}(t)\boldsymbol{x}(t),\quad \boldsymbol{x}(t_0)=\boldsymbol{x}_0 \tag{6}$$

with static output feedback

$$\boldsymbol{u}(t)=\boldsymbol{F}\boldsymbol{y}(t) \tag{7}$$

where

$$\boldsymbol{A}_{CL}(t)\in \mathrm{Co}\{\boldsymbol{A}_{CL1},\ldots,\boldsymbol{A}_{CLN}\}:=\left\{\sum_{i=1}^{N}\alpha_i\boldsymbol{A}_{CLi}:\alpha_i\geq 0,\sum_{i=1}^{N}\alpha_i=1\right\} \tag{8}$$

and

$$\boldsymbol{A}_{\mathrm{CL}i}=\boldsymbol{A}_i+\boldsymbol{B}_i\boldsymbol{F}\boldsymbol{C}_i,\ i=1,\ldots,N \tag{9}$$

The robust static output feedback problem can be formulated as follows. For the system (1) find a static output feedback (7) such that the closed loop system (6) is stable, i.e. eigenvalues of $\boldsymbol{A}_{\mathrm{CL}}$ always have negative real parts. Finding of $\boldsymbol{F}$ is important when the state matrix $\boldsymbol{A}$ is unstable since having $\boldsymbol{F}$ leads to a stabilizing static output feedback.

A sufficient condition for the asymptotic stability of the system (6) is feasibility, e. a. the existence of a quadratic Ljapunov function $V(\boldsymbol{x})=\boldsymbol{x}(t)^T\boldsymbol{P}\boldsymbol{x}(t)$, $\boldsymbol{P}>0$, such that $\frac{\mathrm{d}V(\boldsymbol{x}(t))}{\mathrm{d}t}<0$ along all state trajectories. If a $\boldsymbol{P}>0$ exists, system (6) is quadratically stable and following statement holds: system (6) is quadratically stable if and only if there exists a positive definite matrix $\boldsymbol{P}>0$ such that following inequalities are satisfied

$$\boldsymbol{A}_{\mathrm{CL}i}^T\boldsymbol{P}+\boldsymbol{P}\boldsymbol{A}_{\mathrm{CL}i}^T<0,\ \boldsymbol{P}>0,\ i=1,\ldots,N \tag{10}$$

Consider the uncertain polytopic system (1). Then the following three statements are equivalent (Veselý, 2002).

1. The system (1) is simultaneously static output feedback stabilizable with guaranteed cost J^*

$$\int_0^\infty \left(x(t)^T Q x(t) + u(t)^T R u(t) \right) dt \le x_0(t)^T P x_0(t) = J^*, \; P > 0 \qquad (11)$$

2. There exist matrices $P > 0$, $Q > 0$, $R > 0$ and a matrix F such that the following inequalities hold

$$(A_i + B_i F C_i)^T P + P(A_i + B_i F C_i) + Q + C_i^T F^T R F C_i < 0, \; i = 1,\ldots,N \qquad (12)$$

3. There exist matrices $P > 0$, $Q > 0$, $R > 0$ and a matrix F such that the following inequalities hold

$$A_i^T P + P A_i - P B_i R^{-1} B_i^T P + Q \le 0, \; i = 1,\ldots,N \qquad (13)$$

$$\left(B_i^T P + R F C_i \right) \Phi_i^{-1} \left(B_i^T P + R F C_i \right)^T - R \le 0 \qquad (14)$$

where

$$\Phi_i = -\left(A_i^T P + P A_i - P B_i R^{-1} B_i^T P + Q \right), \; i = 1,\ldots,N \qquad (15)$$

2.2. *Robust static output feedback controller design*

The design procedure for simultaneous static output feedback stabilization of the system (1) with guaranteed cost (11) is based on statements formulated above and their transformation to LMIs. Using Schur complement formula and defining $S = P^{-1}$, the inequality (13) is transformed to the following LMIs

$$\begin{bmatrix} S A_i^T + A_i S - B_i R^{-1} B_i^T & S\sqrt{Q} \\ \sqrt{Q} S & -I \end{bmatrix} < 0, \; \gamma I < S, \; i = 1,\ldots,N \qquad (16)$$

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

The inequality (14) is transformed to the following LMIs

$$\begin{bmatrix} -R & B_i^T P + R F C_i \\ \left(B_i^T P + R F C_i \right)^T & -\Phi_i \end{bmatrix} < 0, \; i = 1,\ldots,N \qquad (17)$$

The algorithm for static output simultaneous stabilization of the system (1) with guaranteed cost (11) is following.

1. Compute $S = S^T > 0$ from the inequalities (16).
2. $P = S^{-1}$.
3. Compute F from the inequalities (17).
4. If the solution of (16) is not feasible, the system (1) is not simultaneously stabilizable by static output feedback. If the solution of (17) is not feasible, the

closed-loop system (6) is not quadratically stable with guaranteed cost. Then it is necessary to change $\boldsymbol{Q}$, $\boldsymbol{R}$ and γ in order to find feasible solutions. If the solutions of (16), (17) are feasible, then the system (1) is simultaneously stabilizable and the system (6) is quadratically stable with guaranteed cost J^* (11).

3. Controlled CSTR

Hydrolysis of propylene oxide to propylene glycol in continuous stirred tank reactor (Molnár et al. 2002) was chosen as a controlled process. The reaction is as follows

$$C_3H_6O + H_2O \rightarrow C_3H_8O_2 \qquad \text{(A)}$$

The reactor with volume of 2.407 m^3 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 the consecutive reactions of propylene oxide with propylene glycol. The reaction is of the first order with respect to propylene oxide as a key component. The dependence of reaction rate constant on temperature is described by Arrhenius equation

$$k = k_{\infty} \exp\left(\frac{-E}{RT_r}\right) \qquad (18)$$

where k_{∞} is pre-exponential factor, E – activation energy, R – gas constant and T_r – temperature of reaction mixture.

Assuming ideal mixing of the reactor and constant volumetric flow rates, the material balance for each component of reaction (A) is

$$V_r \frac{\mathrm{d}c_j}{\mathrm{d}t} = \dot{V}_j\left(c_{j0} - c_j\right) + V_r \nu_j r, \quad j=1,2,3 \qquad (19)$$

where V_r is volume of the reaction mixture, c – molar concentration, $\dot{V}$ – volume flow rate, ν – stoichiometric coefficient, r – molar rate of chemical reaction. Further it is assumed that the coefficients of thermal capacity and volumetric flow rates do not depend on temperature and composition, and also the heat of mixing and mixing volume can be neglected.

The simplified enthalpy balance of reaction mixture used as a standard at reactor design (Ingham et al., 1994) is

$$V_r \rho c_p \frac{\mathrm{d}T_r}{\mathrm{d}t} = \dot{V}\rho c_p\left(T_0 - T\right) - \dot{Q} + V_r\left(-\Delta_r H\right) r \qquad (20)$$

$$\dot{Q} = UA(T_r - T_c) \qquad (21)$$

where T is temperature, ρ – density, c_p – mass heat capacity, $\dot{Q}$ – heat flow rate, $\Delta_r H$ – heat of reaction, U – overall heat transfer coefficient, A – area.

The simplified enthalpy balance of cooling medium used as a standard at reactor design (Ingham et al., 1994) is

$$V_c \rho_c c_{pc} \frac{\mathrm{d}T_c}{\mathrm{d}t} = \dot{V}_c \rho_c c_{pc} (T_{c0} - T_c) + \dot{Q} \qquad (17)$$

Subscripts denote 0 – inlet, c – cooling medium, r – reaction mixture and superscript s – steady state.
Values of parameters and feed values are in Table 1, where c_{10} is the inlet concentration of propylene oxide and c_{30} – inlet concentration of propylene glycol.

$V_r = 2.407\ \mathrm{m^3}$	$\rho = 974.19\ \mathrm{kg\ m^{-3}}$	$T_{r0} = 299.05\ \mathrm{K}$	$\dot{V}^s = 0.072\ \mathrm{m^3\ min^{-1}}$
$V_c = 2\ \mathrm{m^3}$	$\rho_c = 998\ \mathrm{kg\ m^{-3}}$	$T_{c0} = 288.15\ \mathrm{K}$	$\dot{V}_c^s = 0.6307\ \mathrm{m^3\ min^{-1}}$
$c_p = 3.7187\ \mathrm{kJ\ kg^{-1}\ K^{-1}}$	$AU = 120\ \mathrm{kJ\ min^{-1}\ K^{-1}}$	$c_{10} = 0.0824\ \mathrm{kmol\ m^{-3}}$	
$c_{pc} = 4.182\ \mathrm{kJ\ kg^{-1}\ K^{-1}}$	$E/R = 10183\ \mathrm{K}$	$c_{30} = 0\ \mathrm{kmol\ m^{-3}}$	

Table 1: Parameters and steady-state inputs of the chemical reactor

Model uncertainties of the over described reactor follow from the fact that there are two physical parameters in this reactor, heat of reaction and pre-exponential factor, with values known within following intervals:

$$\Delta_r H \in [-8.8\times10^4; -9.4\times10^4],\ k_\infty \in [4.0111\times10^9; 5.4\times10^9] \qquad (22)$$

The nominal values of these parameters are mean values of intervals and they are used for deriving of the nominal model of the CSTR. The minimal and maximal values of intervals are used for obtaining of models, which create the vertex systems for the robust controller design.

4. Simulation results

The steady state behavior of the chemical reactor with nominal values and also with all 4 combinations of minimal and maximal values of 2 uncertain parameters is studied at first. It can be stated the reactor has always three steady states, two of them are stable and one is unstable.

The situation for the nominal model is shown in Fig. 1, where the curve $\dot{Q}_{GEN}$ is the heat generated by the reaction and the line $\dot{Q}_{OUT}$ is the heat withdrawn from the reactor. The steady state operating points of the reactor are points where the curve and the line intersect. The steady states are stable only in the case when the slope of the cooling curve is higher than the slope of the heat generated curve.

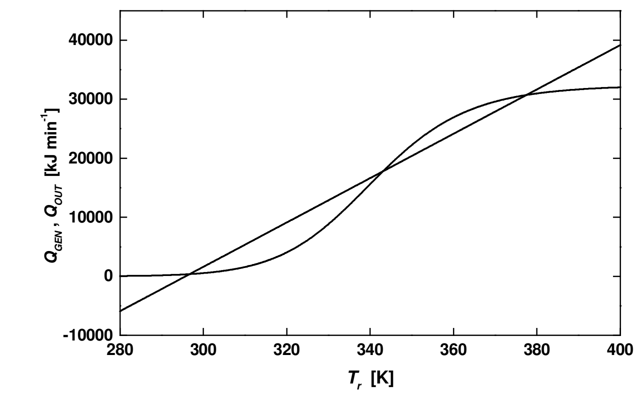

Figure 1: Three steady states of the CSTR with nominal values of uncertain parameters

Further the open-loop behavior of the reactor in its unstable steady state is studied. The main operating point is given by the unstable steady state of the reactor with the temperature of the reaction mixture T_r^s = 343.1K. Simulation results obtained for the nominal model and also for 4 vertex systems are shown in Fig. 2. They confirm that without feedback control, the CSTR cannot operate in its unstable steady state and the CSTR converges either to the upper or to the lower stable steady state.

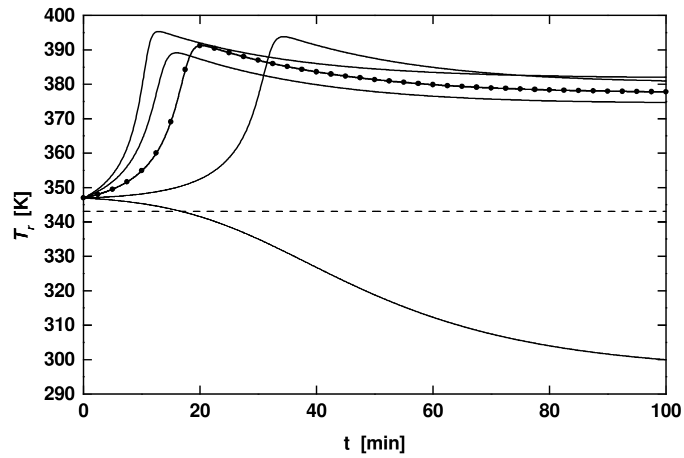

Figure 2: Open-loop response of the CSTR, - - - main operating point, —•—•— nominal system, —— vertex systems

From the viewpoint of safety operation, it is sometimes necessary to stabilize reactors in their unstable steady states. So, the main aim is to stabilize the presented reactor in its unstable steady state. The main operating point is given by the unstable steady-state reactor temperature T_r^s = 343.1K. Because of presence of uncertainties in the CSTR, it is necessary to find a robust stabilizing controller.

Design of a robust stabilizing controller is based on having a linear state space model (1) of the controlled system. Linearized mathematical model of the CSTR has been derived using material balances of propylene oxide and propylene glycol and enthalpy balances of reaction mixture and cooling medium under the assumption that the control inputs are the reaction mixture flow rate $\dot{V}_r$ and the coolant flow rate $\dot{V}_c$. The controlled output is the temperature of reaction mixture T_r. The other input variables are considered to be constant. The matrices of the nominal linearized model in the main operating point are

$$\boldsymbol{A}_0 = \begin{pmatrix} -0.0664 & 0 & -0.0001 & 0 \\ 0.0365 & -0.0299 & 0.0001 & 0 \\ 54.9420 & 0 & 0.1329 & 0.0138 \\ 0 & 0 & 0.0144 & -0.3297 \end{pmatrix}, \quad \boldsymbol{B}_0 = \begin{pmatrix} 0.0188 & 0 \\ -0.0188 & 0 \\ -18.3011 & 0 \\ 0 & -1.1979 \end{pmatrix} \qquad (23)$$

$$\boldsymbol{C}_0 = \begin{pmatrix} 0 & 0 & 1 & 0 \end{pmatrix} \qquad (24)$$

The eigenvalues of $\boldsymbol{A}_0$ are –0.0299, 0.0929, –0.0260, –0.3301 and they confirm the instability of the reactor in one of its steady states. For 2 uncertain parameters, we have obtained also $2^2 = 4$ linearized models, which represent vertices of the uncertain polytopic system and they all are unstable.

It was further important to find a robust static output feedback, which would be able to stabilize the CSTR as the uncertain system with the guaranteed cost expressed by (11), where matrices $\boldsymbol{Q}$, $\boldsymbol{R}$ are chosen as follows

$$\boldsymbol{Q} = q_{const}.\mathrm{diag}(10, 10, 0.001\times10^{-3}, 0.001\times10^{-3}) \qquad (25)$$

$$\boldsymbol{R} = r_{const}.\mathrm{diag}(100, 1\times10^{-4}) \qquad (26)$$

For finding a stabilizing output feedback controller it is necessary to solve two sets of LMIs (16), (17), each set consisting of 4 LMIs. The feasibility of the solution of (16) assures that the reactor is robust static output feedback quadratically stabilizable and the feasibility of the solution of (17) gives robust static output stabilizing controller with guaranteed cost for the whole uncertain system.

For solving the LMIs, the LMI MATLAB toolbox was used. There are three parameters, which influence solution and can be changed: $q_{const}, r_{const}, \gamma$. In dependence on the choice of these parameters, it was possible to find several stabilizing controllers, which stabilize the polytopic system with 4 vertices and also stabilize the reactor. For all stabilizing controllers all closed loop systems obtained for the nominal system and also for 4 vertex systems are stable, e. a. all eigenvalues of state matrices (8) of the nominal and 4 vertex closed loop systems have negative real parts.

Simulation results obtained with the robust static feedback controller $F = \begin{bmatrix} 0.1230 & 10.5575 \end{bmatrix}^T$ are shown in Fig. 3.

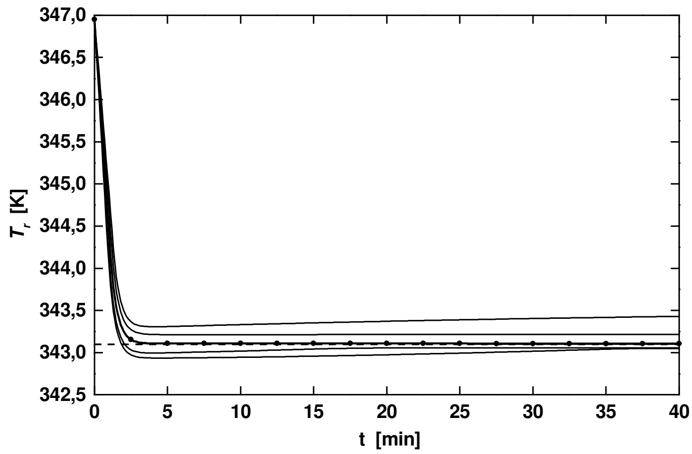

Figure 3: Closed-loop response of the CSTR with the robust output feedback controller, - - - main operating point, —•—•— nominal system, —— vertex systems

Simulations demonstrate also comparison of the designed robust controller with an optimal LQ controller. The optimal LQ controller was designed (Mikleš and Fikar, 2004) with the same matrices Q, R (25), (26) as the robust controller in the form

$$\boldsymbol{K} = \begin{bmatrix} 4.597 & 0.008 & 0.014 & 0.00005 \\ 1803.907 & 8.9023 & 5.211 & 2.9173 \end{bmatrix} \qquad (27)$$

Fig. 4 shows the closed-loop response of the CSTR with the optimal LQ controller. The designed LQ controller is able stabilize the nominal model, but the control response is more sluggish than with the robust controller. The LQ controller is not able to stabilize all vertex systems to the main operating point.

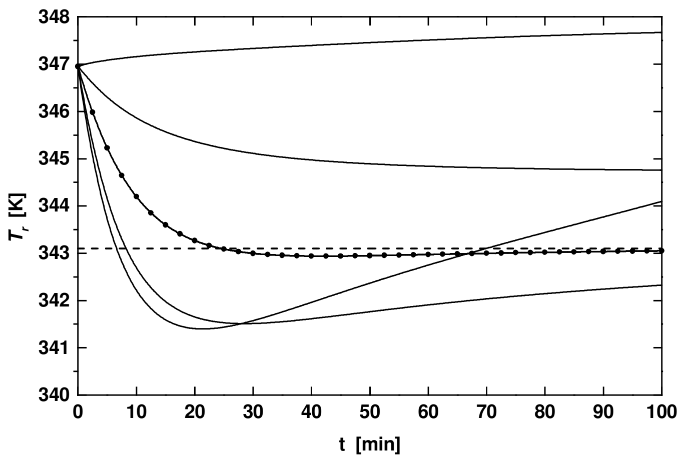

Figure 4: Closed-loop response of the CSTR with the optimal LQ controller, - - - main operating point, —•—•— nominal system, —— vertex systems

5. Conclusions

In this paper, the possibility to stabilize the exothermic chemical reactor for hydrolysis of propylene oxide to propylene glycol with 2 uncertain parameters and multiple steady states via static output feedback controller is studied. The results confirm that using a simple non-iterative algorithm based on solving of two sets of LMIs is a successful way to design robust stabilizing controllers also for such complicated systems as CSTRs with multiple steady states and uncertainties. LQ design gives optimal controllers, which successfully stabilize systems without uncertainties (nominal systems), but they cannot assure stabilization of systems with uncertainties.

6. Acknowledgements

The authors are pleased to acknowledge the financial support of the Scientific Grant Agency of the Slovak Republic under grants No. 1/3081/06 and 1/4055/07.

References

Bakošová, M., Puna, D. and Mészáros, A., *European Symposium on Computer Aided Process Engineering – 15*, Elsevier, Amsterdam, 1303-1308 (2005).

Benton, I.E. and Smith, D., (1999) *Int. J. Control*, 72, 1322-1330.

Boyd, S., L. El Ghaoui, E. F. and Balakrishnan, V., *Linear Matrix Inequalities in System and Control Theory.* SIAM, Philadelphia (1994).

Doyle, J.C. and Stein, G., (1981) *IEEE Trans. Automatic Control*, 26, 4-16.

Gerhard, J., Mönningmann, M. and Marquardt, W., (2004) *Proc. 7th Int. Symp. Dynamics and Control of Process Systems*, Massachusets, No. 92.

Henrion, D., Tarboriech S. and Garcia, G., (1999) *IEEE Trans. Automatic Control*, 44, 2230-2237.

Ingham, J., Dunn, I.J., Heinzle, E. and Přenosil, J.E, *Chemical Engineering Dynamics*, VCH Verlagsgesellschaft, Weinheim, Germany (1994).

Kučera, V. and de Souza, C.E., (1995) *Automatica*, 31, 1357-1359.

Mikleš, J., Fikar, M.: *Process Modelling, Identification, and Control 2*, STU Press, Bratislava, Slovakia (2004).

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

Kuník, S., Mudrončík, D. and Rakovský, M., (2006) *Materials Science and Technology*, (online http://www.mtf.stuba.sk/buxus/generate_page.php?page_id=2450), 6, 1.

Syrmos, V.L., Abdallah, C.T., Dorato, P. and Grigoriadis, K., (1997) , 33, 203-210.

Veselý, V., (2004) *Kybernetika*, 40, 221-232.

Veselý, V., (2002) *Journal of Electrical Engineering*, 53, 117-125.

Zames, G., (1981) *IEEE Trans. Automatic Control*, 26, 301-320.