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Comparison of Robust and Optimal Approach to Stabilisation of CSTRs

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Chemical and biochemical reactors are key plants in chemical and food industry and especially exothermic continuous stirred tank reactors (CSTRs) are very demanding systems. From the control viewpoint some important issues should explored. They include their potential safety problems (Laššák et al., 2010), the possibility of multiple steady states (Moreno et al., 2010), presence of different uncertainties caused by e.g. variation or not exact knowledge of any parameters (Méndez-Acosta et al., 2010), process nonlinearities, changes of operating points. All these problems can cause poor performance of closed-loop control systems with high demands on material and energy consumption.
From economic or safety reasons, it is sometimes necessary to stabilize reactors into their open-loop unstable steady-states (Mjalli and Jayakumar, 2009, Moreno et al., 2010, Savoglidis et al. 2010). Stabilization can lead to significant material and energy savings, especially in the case when the maximum conversion is reached at the temperature that corresponds to the open-loop unstable steady state. This situation is studied in the paper for the CSTR with uncertain parameters. Robust stabilization of the CSTR is designed and it is compared to stabilization using an optimal controller.

1. Controlled CSTR

The controlled process is a CSTR with two 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. Under usual simplifying assumptions (Mikleš and Fikar, 2007), the dynamic mathematical model of the CSTR can be obtained by the mass balances of reactants, the energy balance of the reacting mixture and the energy balance of the coolant in the form of four non-linear differential equations. The parameters are listed in Table 1, where V are volumes, ρ are densities, C_P are specific heat capacities, A_h is the heat transfer area, U is the overall heat transfer coefficient, E are the activation energies, R is the gas constant, c are concentrations, T are temperatures, q are volumetric flow rates, $(\Delta_r H)$ are reaction enthalpies and k_∞ are the pre-exponential factors in the reaction rate constants k. The subscripts denote: r the

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reactant mixture, c the coolant, f feed values, 1 the 1st reaction and 2 the 2nd reaction. The superscript s denotes the steady-state values.

Table 1: Parameters and inputs of the CSTR

variable	unit	value	variable	unit	value
V_r	m^3	0.23	$g_1=E_1/R$	K	9850
V_c	m^3	0.21	$g_2=E_2/R$	K	22019
ρ_r	kg m^{-3}	1020	c_{Af}	kmol m^{-3}	4.22
ρ_c	kg m^{-3}	998	c_{Bf}	kmol m^{-3}	0
C_{Pr}	kJ kg^{-1} K^{-1}	4.02	T_{rf}	K	310
C_{Pc}	kJ kg^{-1} K^{-1}	4.182	T_{cf}	K	288
A_h	m^2	1.51	q_r^s	m^3 min^{-1}	0.015
U	kJ m^{-2} min^{-1} K^{-1}	42.8	q_c^s	m^3 min^{-1}	0.004

The CSTR has 4 parameters which are constant but known only within intervals with minimum and maximum values listed in Table 2. The nominal system is obtained as the model of the reactor with nominal, i.e. mean values of uncertain parameters. The vertex systems are obtained as the models created for all combinations of minimum and maximum values of uncertain parameters and their number is $p = 2^4 = 16$.

Table 2: Uncertain parameters

parameter	unit	minimum value	maximum value
$-(\Delta_r H)_1$	kJ $kmol^{-1}$	8.4×10^4	8.4×10^4
$-(\Delta_r H)_2$	kJ $kmol^{-1}$	5.3×10^4	5.7×10^4
$k_{1\infty}$	min^{-1}	1.5×10^{11}	1.6×10^{11}
$k_{2\infty}$	min^{-1}	4.95×10^{26}	12.15×10^{26}

1.1 Steady-state and open-loop analysis of the CSTR

The steady-state behaviour of the chemical reactor was studied at first. The results obtained for the nominal system (Figure 1a, 1b) and the vertex systems confirmed that the reactor had always three steady states, two of them were stable and one was unstable. The situation for the nominal model is shown in Figure 1a, where Q_{GEN} is the heat generated by chemical reactions and Q_{OUT} is the heat removed by the jacket and the product stream. The reactor works in a steady state when these heats are equal. The maximum concentration of the main product B is obtained at the temperature 338.4 K representing the unstable steady state (Figure 1b). The results of the open-loop analysis confirm that without feedback control the temperature in the reactor converges to the stable steady states with low concentration of B (Figure 1c).

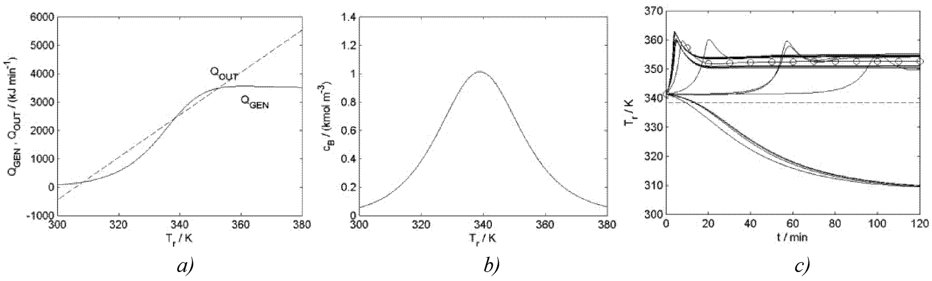

Figure 1: Three steady states of the CSTR (a), dependence of the concentration of the main product on the reacting mixture temperature (b), open-loop behaviour of the nominal model (—o—) and 16 vertex systems (—) (c).

2. Robust static output feedback stabilization of the CSTR

Consider an uncertain linear time invariant (LTI) system in the form

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t), \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \qquad (1)$$
$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{x}(t)$$

where $\boldsymbol{x}(t) \in \mathrm{R}^n$ is the state, $\boldsymbol{u}(t) \in \mathrm{R}^m$ is the control input, $\boldsymbol{y}(t) \in \mathrm{R}^l$ is the controlled output and the polytopic uncertainty is considered. The task is to find a static output feedback controller $\boldsymbol{F}$ with the control law $\boldsymbol{u}(t) = \boldsymbol{F}\boldsymbol{y}(t)$ so that the uncertain LTI closed-loop system (2) is stable. The closed-loop system is again an uncertain LTI polytopic system

$$\dot{\boldsymbol{x}}(t) = \left(\boldsymbol{A} + \boldsymbol{B}\boldsymbol{F}\boldsymbol{C}\right)\boldsymbol{x}(t) = \boldsymbol{A}_{\mathrm{CL}}\boldsymbol{x}(t), \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \qquad (2)$$

$$A_{CL} \in \mathrm{Co}\left\{\boldsymbol{A}_{CL1}, \ldots, \boldsymbol{A}_{CLp}\right\} = \left\{\sum_{i=1}^{p} \alpha_i \boldsymbol{A}_{CLi} : \alpha_i \geq 0, \sum_{i=1}^{p} \alpha_i = 1\right\}, \boldsymbol{A}_{CLi} = \boldsymbol{A}_i + \boldsymbol{B}_i \boldsymbol{F}\boldsymbol{C}_i \qquad (3)$$

The system (1) is simultaneously stabilisable using static output feedback $\boldsymbol{u}(t) = \boldsymbol{F}\boldsymbol{y}(t)$ with guaranteed cost

$$J = \int_0^{\infty} \left(\boldsymbol{x}(t)^T \boldsymbol{Q}\boldsymbol{x}(t) + \boldsymbol{u}(t)^T \boldsymbol{R}\boldsymbol{u}(t)\right) \mathrm{d}t \leq \boldsymbol{x}_0(t)^T \boldsymbol{P}\boldsymbol{x}_0(t) = J^* \qquad (4)$$

if there exist matrices $\boldsymbol{P} = \boldsymbol{P}^T > 0$, $\boldsymbol{Q} > 0$, $\boldsymbol{R} > 0$ and $\boldsymbol{F}$ such that the following inequalities hold (Veselý, 2006)

$$\boldsymbol{A}_i^T \boldsymbol{P} + \boldsymbol{P}\boldsymbol{A}_i - \boldsymbol{P}\boldsymbol{B}_i \boldsymbol{R}^{-1} \boldsymbol{B}_i^T \boldsymbol{P} + \boldsymbol{Q} \leq 0, \quad i = 1, \ldots, p \qquad (5)$$

$$\left(\boldsymbol{B}_i^T \boldsymbol{P} + \boldsymbol{R}\boldsymbol{F}\boldsymbol{C}_i\right) \boldsymbol{\Phi}_i^{-1} \left(\boldsymbol{B}_i^T \boldsymbol{P} + \boldsymbol{R}\boldsymbol{F}\boldsymbol{C}_i\right)^T - \boldsymbol{R} \leq 0, \quad i = 1, \ldots, p \qquad (6)$$

where

$$\boldsymbol{\Phi}_i = -\left(\boldsymbol{A}_i^T \boldsymbol{P} + \boldsymbol{P}\boldsymbol{A}_i - \boldsymbol{P}\boldsymbol{B}_i \boldsymbol{R}^{-1} \boldsymbol{B}_i^T \boldsymbol{P} + \boldsymbol{Q}\right) \tag{7}$$

2.1 Design procedure

The design procedure is based on matrix inequalities (5) – (7). Use Schur complement transforms (5) – (7) to linear matrix inequalities (LMIs) (8), (9).

1st Step: compute $\boldsymbol{S} = \boldsymbol{S}^T > 0$ from the 1st set of LMIs

$$\begin{bmatrix} \boldsymbol{S}\boldsymbol{A}_i^T + \boldsymbol{A}_i\boldsymbol{S} - \boldsymbol{B}_i\boldsymbol{R}^{-1}\boldsymbol{B}_i^T & \boldsymbol{S}\sqrt{\boldsymbol{Q}} \\ \sqrt{\boldsymbol{Q}}\boldsymbol{S} & -\boldsymbol{I} \end{bmatrix} \le 0\,,\ \gamma\boldsymbol{I} < \boldsymbol{S}\,,\ i = 1,\ldots,p \tag{8}$$

where $\gamma > 0$ is any non-negative constant and $\boldsymbol{S} = \boldsymbol{P}^{-1}$.

2nd Step: compute $\boldsymbol{F}$ from the 2nd set of LMIs

$$\begin{bmatrix} -\boldsymbol{R} & \boldsymbol{B}_i^T\boldsymbol{P} + \boldsymbol{R}\boldsymbol{F}\boldsymbol{C}_i \\ \left(\boldsymbol{B}_i^T\boldsymbol{P} + \boldsymbol{R}\boldsymbol{F}\boldsymbol{C}_i\right)^T & -\boldsymbol{\Phi}_i \end{bmatrix} \le 0\,,\ i = 1,\ldots,p \tag{9}$$

If the solutions of (8), (9) are not feasible, either the system (1) is not stabilisable with a prescribed guaranteed cost, or it is necessary to change $\boldsymbol{Q}$, $\boldsymbol{R}$ or γ in order to find a feasible solution.

3. Optimal control

Linear quadratic regulator (LQR) problem can be formulated as the task to find the controller $\boldsymbol{K}$ described by the control law $\boldsymbol{u}(t) = \boldsymbol{K}\boldsymbol{x}(t)$ so that the quadratic cost function J (4) is minimised. The optimal gain is $\boldsymbol{K} = -\boldsymbol{R}^{-1}\boldsymbol{B}^T\boldsymbol{P}$ and $\boldsymbol{P} = \boldsymbol{P}^T > 0$ is a solution of the matrix Riccati equation (Mikleš and Fikar, 2007)

$$\boldsymbol{A}_0^T\boldsymbol{P} + \boldsymbol{P}\boldsymbol{A}_0 - \boldsymbol{P}\boldsymbol{B}_0\boldsymbol{R}^{-1}\boldsymbol{B}_0^T\boldsymbol{P} + \boldsymbol{Q} = 0 \tag{10}$$

where the subscript 0 means that the LQR problem is solved for the deterministic system, which can be the represented by the nominal model.

4. Simulation results

Design of both, the robust and the LQ controller is based on having a linear state space model of the CSTR. The linear model was derived using standard linearisation technique under the assumption that the control inputs are the reacting mixture flow rate q_r and the coolant flow rate q_c and the controlled outputs are the temperature of the reacting mixture T_r in the reactor and the temperature of coolant T_c in the jacket. The controlled variables were stabilised to the values representing the open-loop unstable steady state T_r^s=338.4 K and T_c^s=328.1 K. Using the technique described in Sections 2 and 3 it was possible to find several robust and LQ controllers. The results are presented for the controllers

$$F = \begin{pmatrix} 0.0320 & 0.0058 \\ 0.0108 & 0.0041 \end{pmatrix}, \quad K = \begin{pmatrix} 0.0084 & 0.0004 & 0.0048 & 0.0004 \\ 0.0061 & -0.0006 & 0.0012 & 0.0028 \end{pmatrix} \tag{11}$$

The controllers were found for the weight matrices $\boldsymbol{Q}$ = diag(0.1, 0.1,0.01, 0.01), $\boldsymbol{R}$ = diag (1000, 1000) in (4) and variable $\gamma = 0.01$ in Eq (8).
Figures 2 and 3 compare the stabilisation of the CSTR using the robust $\boldsymbol{F}$ and the optimal controller $\boldsymbol{K}$. The values of the cost function J (4), the received concentration c_B of the main product B and the volume of the cold water V_c consumed during the stabilization were also followed for all simulated systems. The worst values of these parameters J_{max}, $c_{B,min}$ and $V_{c,max}$ are listed in Table 3. All these parameters are better when the robust controller was used for stabilisation.

Table 3: Comparison of robust and optimal controller

Controller	$J_{\max}$	$V_{c,\max}$ / m^3	$c_{B,min}$ / kmol m^{-3}
robust	4.9561	0.2891	1.6965
optimal	12.9589	0.3299	1.6634

5. Conclusions

Obtained results confirm that using the robust controller for stabilisation of reactors with uncertain parameters can assure the higher production of the main product and the smaller consumption of coolant in comparison to LQ controller. The LQ controller is optimal for the system without uncertainty, but the controller is not able to assure optimal performance of the uncertain system. Implementation of robust control in industrial application can lead to significant energy savings.

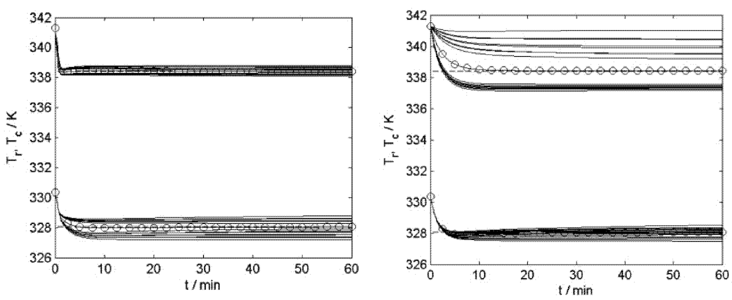

Figure 2: Stabilisation of the CSTR using robust (left) and LQ (right) controller: controlled outputs of the nominal model (—o—) and 16 vertex systems (—)

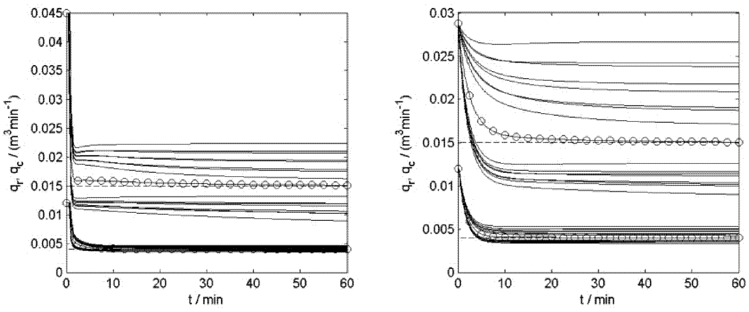

Figure 3: Stabilisation of the CSTR using robust (left) and LQ (right) controller: control inputs of the nominal model (—o—) and 16 vertex systems (—)

Acknowledgments

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