SIMULATION OF ROBUST STABILIZATION OF A CHEMICAL REACTOR

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CSTR, multiple steady states, stabilization, static output feedback, PID controller.

ABSTRACT
The paper presents simulation experiments on the continuous stirred tank reactor for hydrolysis of propylene oxide to propylene glycol. The reactor is exothermic one. There are two parameters with only approximately known values in the reactor. These parameters are the reaction rate constant and the reaction enthalpy. The simplified mathematical model of the reactor consists of four nonlinear ordinary differential equations. The steady state analysis shows the reactor has multiple steady states and the open-loop analysis confirms that the reactor is open-loop unstable around one of these steady states. Then the possibility to stabilize the reactor using static output feedback PI and PID controllers is studied. Because of the presence of uncertainty in the continuous stirred tank reactor, the robust static output feedback is designed. Simulations are used for testing the stabilizability of the reactor around its open-loop unstable steady state.

INTRODUCTION
Continuous stirred tank reactors (CSTRs) are often used plants in chemical industry and especially exothermic CSTRs are very interesting systems from the control viewpoint because of their potential safety problems and the possibility of exotic behaviour such as multiple steady states, see e.g. (Molnár et al., 2002), (Pedersen and Jørgensen, 1999). 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. reaction rate constants, reaction enthalpies and heat transfer coefficients (Antonelli and Astolfi, 2003). The other control problems are due to the high sensitivity of the state and output variables to input changes and process nonlinearities (Alvarez-Ramirez and Femat, 1999). Operating points of reactors change in other cases. In addition, the dynamic characteristics may exhibit a varying sign of the gain in various operating points. All these problems can cause poor performance or even instability of closed-loop control systems.

Conventional control strategies, which are often used for reactor control design, can fail for such complicated systems and their effective control requires application some of advanced methods, as e.g. adaptive control (Vojtesek and Dostal, 2008), predictive control (Figueroa et al., 2007), robust control (Alvarez-Ramirez and Femat, 1999), (Gerhard et al., 2004), (Bakosová et al., 2005), (Tlacuahuac et al., 2005) and others.

Robust control has grown as one of the most important areas in modern control design since works by (Doyle and Stein, 1981), (Zames and Francis, 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. (Syrmos et al., 1997), (Antonelli and Astolfi, 2003). 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. Especially, 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 et al., 1994) and references therein.

From the system theory viewpoint, CSTRs belong to a class of nonlinear lumped parameter systems. Their mathematical models are described by sets of nonlinear ordinary differential equations (ODEs). The methods of modelling and simulation of such processes are described e.g. in (Ingham et al., 1994). The models are often used for a preliminary analysis of the steady-state, open-loop and closed-loop behaviour of chemical reactors.

The paper presents simulation experiments with the CSTR for hydrolysis of propylene oxide to propylene glycol. The reactor is exothermic one. There are two parameters with only approximately known values in the reactor. The steady state analysis shows that the reactor has multiple steady states and the open-loop analysis confirms that the reactor is open-loop unstable around one of these steady states. Then the possibility to stabilize the reactor using robust static output feedback PI and PID controllers is studied by simulations.
MODEL OF THE CSTR

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

\[
\text{C}_3\text{H}_4\text{O} + \text{H}_2\text{O} \rightarrow \text{C}_3\text{H}_6\text{O}_2
\]  

(1)

The reaction is of the first order with respect to propylene oxide as a key component. The dependence of the reaction rate constant on the temperature is described by the Arrhenius equation

\[
k = k_\infty e^{-\frac{E_a}{RT}}
\]  

(2)

where \(k_\infty\) is the pre-exponential factor, \(E_a\) is the activation energy, \(R\) is the universal gas constant and \(T\) is the temperature of the reaction mixture. Assuming ideal mixing in the reactor, the constant reaction volume and the same volumetric flow rates of the inlet and outlet streams, the mass balance for any component \(j\) in the system is

\[
V_r \frac{dc_j}{dt} = q_r (c_{j0} - c_j) + \nu_j rV_r,
\]  

(3)

where \(V_r\) is the reaction volume, \(c\) is the molar concentration, \(q\) is the volumetric flow rate, \(\nu\) is the stoichiometric coefficient, \(r\) is the molar rate of the chemical reaction and subscripts denote \(j\) the component, \(r\) the reaction mixture, \(0\) the feed. It is assumed further that the specific heat capacities, densities and volumetric flow rates do not depend on temperature and composition, and also the heat of mixing and the mixing volume can be neglected. The simplified enthalpy balance of the reaction mixture used as a standard at reactor design (Ingham et al., 1994) is

\[
V_r \rho_r C_P \frac{dT_r}{dt} = q_r \rho_r C_P \left( T_{r0} - T_r \right) - U A \left( T_r - T_c \right) + rV_r (\Delta_r H)^o
\]  

(4)

and the simplified enthalpy balance of the cooling medium is

\[
V_c \rho_c C_p \frac{dT_c}{dt} = q_c \rho_c C_p \left( T_{c0} - T_c \right) + U A \left( T_r - T_c \right)
\]  

(5)

where \(T\) is the temperature, \(\rho\) is the density, \(C_P\) is the specific heat capacity, \((-\Delta_r H)^o\) is the reaction enthalpy, \(U\) is the overall heat transfer coefficient and \(A\) 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 CSTR are summarized in Table 1.

Model uncertainties of the over described reactor follow from the fact that there are two physical parameters in this reactor, the reaction enthalpy and the pre-exponential factor, which values are known within following intervals (Table 2). The nominal values of these parameters are mean values of the intervals and they are used for deriving of the nominal model of the CSTR. The minimal and maximal values of the intervals are used for obtaining models, which create the vertex systems (7).

### Table 1: Constant parameters and steady-state inputs of the CSTR

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V_r)</td>
<td>2.407</td>
<td>m³</td>
</tr>
<tr>
<td>(V_c)</td>
<td>2</td>
<td>m³</td>
</tr>
<tr>
<td>(\rho_r)</td>
<td>947.19</td>
<td>kg m⁻³</td>
</tr>
<tr>
<td>(\rho_c)</td>
<td>998</td>
<td>kg m⁻³</td>
</tr>
<tr>
<td>(C_{P_r})</td>
<td>3.7187</td>
<td>kJ kg⁻¹ K⁻¹</td>
</tr>
<tr>
<td>(C_{P_c})</td>
<td>4.182</td>
<td>kJ kg⁻¹ K⁻¹</td>
</tr>
<tr>
<td>(AU)</td>
<td>120</td>
<td>kJ min⁻¹ K⁻¹</td>
</tr>
<tr>
<td>(E_a/R)</td>
<td>10183</td>
<td>K</td>
</tr>
<tr>
<td>(q_r)</td>
<td>0.072</td>
<td>m³ min⁻¹</td>
</tr>
<tr>
<td>(q_c)</td>
<td>0.6307</td>
<td>m³ min⁻¹</td>
</tr>
<tr>
<td>(c_{C_3H_6O,0})</td>
<td>0.0824</td>
<td>kmol m⁻³</td>
</tr>
<tr>
<td>(c_{C_3H_6O_2,0})</td>
<td>0</td>
<td>kmol m⁻³</td>
</tr>
<tr>
<td>(T_{r0})</td>
<td>299.05</td>
<td>K</td>
</tr>
<tr>
<td>(T_{c0})</td>
<td>288.15</td>
<td>K</td>
</tr>
</tbody>
</table>

### Table 2: Uncertain parameters of the CSTR

<table>
<thead>
<tr>
<th>Parameter</th>
<th>((-\Delta_r H)^o)</th>
<th>(k_\infty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unit</td>
<td>kJ kmol⁻¹</td>
<td>min⁻¹</td>
</tr>
<tr>
<td>Minimal Value</td>
<td>(-5.28 \times 10^6)</td>
<td>(-2.4067 \times 10^{11})</td>
</tr>
<tr>
<td>Maximal Value</td>
<td>(-5.64 \times 10^6)</td>
<td>(-3.2467 \times 10^{11})</td>
</tr>
</tbody>
</table>

### STEADY-STATE AND OPEN-LOOP ANALYSIS

The steady-state model of the CSTR in the form of a set of nonlinear algebraic equations (AEs) is obtained from the dynamic model (3)–(5) equating the derivative terms to zero. MATLAB function `fsolve` can be used for solving the set of nonlinear AEs. The steady state behaviour of the chemical reactor with nominal values and also with 4 combinations of minimal and maximal values of 2 uncertain parameters was 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 is shown in Figure 1, where the curve \(Q_{GEN}\) (the curve is marked with * for the nominal model) represents the heat generated by the reaction and the line \(Q_{OUT}\) is the heat withdrawn from the reactor. The steady states of the reactor are points, where the curves and the line intersect. The steady states are stable if the slope of the cooling line is higher than the slope of the heat generated curve. This condition is satisfied for the nominal model at \(T_r = 296.7\) K and \(T_r = 377.5\) K, and is not satisfied at \(T_r = 343.1\) K.

From the viewpoint of safety operation or in the case when the unstable steady-state coincides with the point that yields the maximum reaction rate at a prescribed temperature, it can be necessary to control a CSTR about its open-loop unstable steady-state, see e. g. (Pedersen and Jørgensen, 1999), (Antonelli and Astolfi, 2003),
which represent vertices of (6) and matrices $A$, $B$, $C$ are convex envelopes of matrices $A_i$, $B_i$, $C_i$, respectively, $i = 1, \ldots, N$. The number of vertex systems $N = 2^p$, where $p$ is the number of uncertain parameters of (6).

**Static Output Feedback With P Controller**

Assume that it is necessary to find for the system (6) a static output feedback

$$u(t) = Fy(t)$$  \hspace{1cm} (8)

with $F \in \mathbb{R}^{m \times r}$ such that the closed loop system

$$\dot{x}(t) = (A + BFC)x(t) = A_{CL}x(t)$$  \hspace{1cm} (9)

is stable, i.e. eigenvalues of $A_{CL}$ have negative real parts. Finding of $F$ is important when the state matrix $A$ is unstable since having $F$ leads to a stabilizing static output feedback.

But the output feedback (8) does not have integral action. One way of forcing an integral action to the output feedback is to put a set of integrators at the output of the plant, see e.g. Mikleš et al. (2006), Puna and Bakošová (2007). Forcing of derivative action to the output feedback has analogous basement.

**Static output feedback with PI controller**

For the system (6), it is necessary to find a static output feedback

$$u(t) = F_1y(t) + F_2 \int_0^t y(\tau)d\tau$$  \hspace{1cm} (10)

with $F_1, F_2 \in \mathbb{R}^{m \times r}$.

Define a new state $z(t) = [z_1(t), z_2(t)]^T$, where $z_1(t) = x(t)$ and $z_2(t) = \int_0^t y(\tau)d\tau$. The dynamics of the newly defined system can be described as follows

$$\dot{z}_1(t) = \dot{x}(t) = Az_1(t) + Bu(t), \quad x_0$$  \hspace{1cm} (11)

$$\dot{z}_2(t) = y(t) = Cz_1(t)$$  \hspace{1cm} (12)

or

$$\dot{z}(t) = \overline{A}z(t) + \overline{B}u(t),$$  \hspace{1cm} (13)

where

$$\overline{A} = \begin{pmatrix} A & 0 \\ C & 0 \end{pmatrix}, \quad \overline{B} = \begin{pmatrix} B \\ 0 \end{pmatrix}.$$  \hspace{1cm} (14)

The output of the newly defined system is described as follows

$$\overline{y}(t) = \overline{C}z(t),$$  \hspace{1cm} (15)

where

$$\overline{C} = \begin{pmatrix} C & 0 \\ 0 & I \end{pmatrix}.$$  \hspace{1cm} (16)

with $I \in \mathbb{R}^{r \times r}$.
So, the design of a static output feedback PI controller (10) can be transformed to the design of a static output feedback P controller

\[ F = [F_1 \quad F_2] \]  

for the system (13) and (15).

**Static output feedback with PID controller**

For the system (6), it is necessary to find a static output feedback

\[ u(t) = F_1 y(t) + F_2 \int_0^t y(\tau) d\tau + F_3 \frac{dy(t)}{dt} \]  

with \( F_1, F_2, F_3 \in \mathbb{R}^{n \times r} \).

Define again a new state \( z(t) = [z_1^T(t), z_2^T(t)]^T \), where \( z_1(t) = x(t) \) and \( z_2(t) = \int_0^t y(\tau) d\tau \). Use \( z(t) \) and (6) leads to

\[ y(t) = C z_1(t) = (C \quad 0) z(t) \]  

\[ \int_0^t y(\tau) d\tau = z_2(t) = (0 \quad I) z(t) \]  

\[ \frac{dy(t)}{dt} = C \dot{z} = CAx(t) + CBu(t) = (CA \quad 0) z(t) + CBu(t) \]  

After the substitution (19), (20) and (21) into (18) and under the assumption that the matrix \( F_4 = (I - F_3CB)^{-1} \) exists, we obtain

\[ u(t) = \bar{F}_1 \overline{y}_1(t) + \bar{F}_2 \overline{y}_2(t) + \bar{F}_3 \overline{y}_3(t) \]  

where \( \overline{y}_1(t) = \overline{C}_i z(t) \), \( i = 1, 2, 3 \), \( \overline{C}_1 = (C \quad 0) \), \( \overline{C}_2 = (0 \quad I) \), \( \overline{C}_3 = (CA \quad 0) \), \( \overline{F}_1 = F_4 \overline{F}_1 \), \( \overline{F}_2 = F_4 \overline{F}_2 \) and \( \overline{F}_3 = F_4 \overline{F}_3 \).

Defining

\[ \bar{F} = (\bar{F}_1 \quad \bar{F}_2 \quad \bar{F}_3) \]  

\[ \bar{y}(t) = (\overline{y}_1^T(t) \overline{y}_2^T(t) \overline{y}_3^T(t))^T \]  

\[ \overline{C} = (\overline{C}^T_1 \overline{C}^T_2 \overline{C}^T_3)^T \]  

we obtain a new dynamic system

\[ \dot{z}(t) = \overline{A} z(t) + \overline{B} u(t) \]  

\[ \bar{y}(t) = \overline{C} z(t) \]  

with

\[ u(t) = \bar{F} \bar{y}(t) \]  

and

\[ \overline{A} = \begin{pmatrix} A & 0 \\ C & 0 \end{pmatrix}, \quad \overline{B} = \begin{pmatrix} B \\ 0 \end{pmatrix}, \quad \overline{C} = \begin{pmatrix} C & 0 \\ 0 & I \\ CA & 0 \end{pmatrix} \]

So, the design of a static output feedback PID controller is transformed to the design of a static output feedback P controller for the system (26). After finding the P controller \( \bar{F} = (\bar{F}_1 \quad \bar{F}_2 \quad \bar{F}_3) \), we obtain the PID controller

\[ F = [F_1 \quad F_2 \quad F_3] \]  

as follows

\[ F_3 = (\bar{F}_3(I + CB\bar{F}_3))^{-1} \]  

\[ F_2 = (I - F_3CB)\bar{F}_2 \]  

\[ F_1 = (I - F_3CB)\bar{F}_1 \]

**Robust static output feedback controller design**

Consider an uncertain polytopic closed-loop system with the system (6) and one of static output feedback controllers (8), (17) and (28). The closed-loop system is described

\[ \dot{x}(t) = [A + BFC] x(t) = A_{CL} x(t) \]  

where \( A_{CL} \) is a convex envelope of a set of linear time invariant matrices \( A_{CLi} \)

\[ A_{CLi} = A_i + B_i FC_i, \quad i = 1, \ldots, N \]  

System (32) is quadratically stable if and only if there exists a positive definite matrix \( P > 0 \) such that following inequalities hold

\[ A_{CLi}^T P + PA_{CLi} < 0, \quad P > 0, \quad i = 1, \ldots, n \]  

Consider the uncertain polytopic system (6). Two following statements are equivalent according to Veselý (2002).

1. The system (32) is simultaneously static output feedback stabilizable with guaranteed cost \( J^* \)

\[ \int_0^\infty [x(t)^T Q x(t) + u(t)^T R u(t)] dt \leq x_0^T P x_0 < J^*, \quad P > 0 \]  

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

\[ A_i^T P + P A_i - PB_i R^{-1} B_i^T P \leq Q, \quad i = 1, \ldots, n \]  

\[ (B_i^T P + R F C_i) \phi_i^{-1}(B_i^T P + R F C_i)^T \leq R \quad i = 1, \ldots, n \]

where

\[ \phi_i = (A_i^T P + P A_i - PB_i R^{-1} B_i^T P + Q), \quad i = 1, \ldots, n \]

The second statement is used for the design of a static feedback controller for simultaneous stabilization of the system (32) with guaranteed cost (35) (Veselý, 2002). Using the Schur complement and defining \( S = P^{-1} \), the inequality (36) is transformed to the following LMIs

\[ \begin{bmatrix} S A_i^T + A_i S - B_i R^{-1} B_i^T S \sqrt{Q} & S \sqrt{Q} \\ \sqrt{Q}^T & -I \end{bmatrix} \leq 0, \quad i = 1, \ldots, n \]
where $\gamma > 0$ is any non-negative constant.

Using $P = S^{-1}$, the inequality (37) can be rewritten to the following LMIs

$$
\begin{bmatrix}
-R & B_i^T P + RFC_i \\
(B_i^T P + RFC_i)^T & -\phi_i
\end{bmatrix} \leq 0
$$

The algorithm has the following steps.

1. Compute $S = S^T > 0$ from the LMIs (39).
2. $P = S^{-1}$.
3. Compute $F$ from the LMIs (40).
4. If the solution of (39) is not feasible, the system (32) is not simultaneously stabilizable by a static output feedback. If the solution of (40) is not feasible, the closed-loop system (32) is not quadratically stable with guaranteed cost. Then change $Q, R$ or $\gamma$ in order to find feasible solutions.

There are two parameters in the presented algorithm, which can be called tuning parameters. They are weighting matrices $Q$ and $R$ in (35). The choice of $\gamma$ in (39) also influences the solution, but $\gamma$ is only a LMI variable.

**ROBUST STABILIZATION OF THE CSTR**

The main aim was to study possibility to stabilize the described CSTR around the open-loop unstable steady state at the temperature $T_r = 343.1$ K using static output feedback PI and PID controllers.

It was necessary to obtain a linear state space model (6) of the controlled process at first. The model was derived using linearization of non-linear terms in the mathematical model (3)–(5). The working point for linearization was the unstable steady state. It was supposed for control purposes that the reactor was the two-input single-output system. The reaction mixture flow rate $q_r$ and the coolant flow rate $q_c$ were chosen as the control inputs and the temperature of the reaction mixture $T_r$ was selected as the controlled output. For 2 uncertain parameters, we obtained one nominal system and $2^2 = 4$ vertex systems (7). All these systems were unstable.

For finding stabilizing output feedback PI or PID controllers, it was necessary to solve two sets of LMIs (39), (40), each set consisting of 4 LMIs. The feasibility of the solution of (39) assured that the reactor was robust static output feedback quadratically stabilizable and the feasibility of the solution of (40) gave robust static output stabilizing controller with guaranteed cost for the whole uncertain system. For solving of LMIs, the LMI MATLAB Toolbox was used. Following parameters influenced solution and could be changed: $Q, R, \gamma$. In dependence on the choice of these parameters, it was possible to find several stabilizing PI and PID controllers. Two of them are presented in Table 3 and they were obtained with

$$
Q = \text{diag } (27, 27, 9 \times 10^{-7}, 9 \times 10^{-7}, 9 \times 10^{-6})
$$

$$
R = \text{diag } (9 \times 10^{-3}, 9 \times 10^{-4}), \quad \gamma = 5 \times 10^{-6}
$$

<p>| Values of elements of $Q$ and $R$ were chosen with respect to the values of state and input variables. |</p>
<table>
<thead>
<tr>
<th>Table 3: Stabilizing PI and PID controllers</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PI</strong></td>
</tr>
</tbody>
</table>
| $F_1$ | $\begin{bmatrix}
3.08 \times 10^{-2} \\
5.43 \times 10^{-1}
\end{bmatrix}$ | $\begin{bmatrix}
9.71 \times 10^{-2} \\
4.89
\end{bmatrix}$ |
| $F_2$ | $\begin{bmatrix}
8.51 \times 10^{-3} \\
2.24 \times 10^{-1}
\end{bmatrix}$ | $\begin{bmatrix}
3.53 \times 10^{-2} \\
1.83
\end{bmatrix}$ |
| $F_3$ | $\begin{bmatrix}
1.43 \times 10^{-2}
\end{bmatrix}$ | $\begin{bmatrix}
3.65
\end{bmatrix}$ |

The possibility to stabilize the reactor using designed robust static output feedback PI and PID controllers was studied by simulations. The nonlinear model of the CSTR was used as the controlled system and the initial temperature of the reaction mixture was $T_r(0) = 346.95$ K. The aim was to control the temperature in the CSTR about the value $T_s = 343.1$ K. The control input boundaries were as follows: $q_r \in [0; 0.18]$ m$^3$min$^{-1}$ and $q_c \in [0; 1.58]$ m$^3$min$^{-1}$. Following disturbances in the feed temperature of the reaction mixture were loaded: $T_{r_0}$ increased by 4 K for $t \in [20; 70]$ min and decreased by 8 K for $t \in [70; 100]$ min. Obtained simulation results are shown in Figures 3, 4. Both, PI and PID static output feedback controllers are able to stabilize the CSTR with uncertainties about its open-loop unstable steady state. The robust PID controller attenuates disturbances very fast and the overshoots caused by disturbances are minimal.

![Figure 3: Robust PI stabilization of the CSTR - controlled output](image-url)
CONCLUSION

In this paper, the possibility to use simulations for steady-state, open-loop and closed-loop analysis of the CSTR for hydrolysis of propylene oxide to propylene glycol was studied. The main aim was to study the possibility to stabilize the exothermic CSTR with uncertain parameters using static output feedback PI and PID controllers. The non-iterative algorithm for design of robust static output feedback PID like controllers is presented. The design of robust controllers is based on solution of LMI, for which the MATLAB LMI Toolbox can be successfully used. Simulations confirmed that robust static output feedback PI or PID controllers can be successfully used for control of CSTRs with multiple steady states, uncertainties and disturbances, even though CSTRs are very complicated systems from the control point of view. The advantage of robust PI and PID controllers is that they do not retain steady-state control errors and they both are able stabilize the open-loop unstable processes. All simulations were done using MATLAB 6.5.

ACKNOWLEDGEMENT

The work has been supported by the Scientific Grant Agency of the Slovak Republic under grants No.1/4055/07 and 1/0071/09. This support is very gratefully acknowledged.

Figure 4: Robust PID stabilization of a CSTR - controlled output

Figure 6: Robust PI stabilization of the CSTR with disturbances and noisy signals - control input $q_r$

Figure 8: Robust PID stabilization of the CSTR with disturbances and noisy signals - controlled output

Figure 9: Robust PID stabilization of the CSTR with disturbances and noisy signals - control input $q_r$

Figure 5: Robust PI stabilization of the CSTR with disturbances and noisy signals - controlled output

Figure 7: Robust PI stabilization of the CSTR with disturbances and noisy signals - control input $q_c$
REFERENCES


AUTHOR BIOGRAPHIES

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