$\mathcal{H}_2$ optimal control of a chemical reactor

Ján Mikleš, Ľuboš Čirka, and Miroslav Fikar

Abstract—**This paper deals with $\mathcal{H}_2$ control of a continuous stirred tank reactor (CSTR). The coolant temperature and the temperature in the reactor are respectively considered as control and controlled variables. A connection between $\mathcal{H}_2$ polynomial approach and the mixed sensitivity optimization for feedback control of CSTR is presented. The control algorithm has been implemented with the help of the Polynomial Toolbox for MATLAB. Simulation results demonstrate the robustness properties of $\mathcal{H}_2$ control of CSTR.**

Keywords—**$\mathcal{H}_2$ optimal control, controller with integral action, chemical reactor.**

I. Introduction

TRADITIONALLY linear methods have been used to design controllers for CSTRs. Control schemes, that have been proposed, include conservative linear controllers and linear controllers with gain scheduling. These methods are based on the first-order approximation of the actual system at a single point and a discrete set of operating points, respectively. Consequently, these techniques cannot account for large perturbations or operation away from the steady-state operating curve.

There are various design methods, which utilize more accurate nonlinear models. A precise treatment of model nonlinearities has emerged for example with the differential geometric techniques of linearization [1]. These methods have been applied to the aforementioned CSTR problem to obtain exact state linearization, exact input-output linearization and state linearization with disturbance rejection. The major shortcoming of these techniques is their lack of robustness guaranties.

The problem of robust stability of closed loop systems has received a considerable amount of attention in recent years. In particular, $\mathcal{H}_2$ and $\mathcal{H}_\infty$ approaches to optimal control design and loop shaping has provided some promising results in the area of robust stabilization of plants.

The modern control area is usually believed to span the period from 1960 to 1980. This coincided with the introduction of state-space-based synthesis techniques. These state-space approaches were thought as being time-domain methods, although Parseval's theorem enabled the control problem to be posed equally well in frequency domain (classical approach). At the present time, $\mathcal{H}_\infty$ optimal control is employed both in the state-space [2] as well as with the polynomial methods [3].

In $\mathcal{H}_\infty$ loop shaping design it is necessary to model plant uncertainty of the nominal plant.

Chemical reactors (CSTR) are commonly used in the process industries. The reactor is a nonlinear process with time-varying parameters. It is necessary to control these reactors to improve their behavior. Usually, input-output models are used for control purposes. These models only represent an approximation of the considered CSTR dynamics. In fact, the CSTR parameters can be varying. Then it is necessary to implement robust control strategies for improving the behavior of the CSTR. $\mathcal{H}_\infty$ optimization of CSTR control deals with the minimization of the peak value of certain closed-loop frequency response functions.

It can be seen, that $\mathcal{H}_2$ optimization with shaping is the $\mathcal{H}_2$ version of the well-known mixed sensitivity problem of $\mathcal{H}_\infty$ optimization [4]. Therefore, robust control algorithms can be based on $\mathcal{H}_2$ optimal control.

In this paper control of a chemical reactor is studied. Control design is based on $\mathcal{H}_2$ optimal control design. The resulting controller has integral action.

The rest of the paper is organized as follows. Section 2 is devoted to the formulation of $\mathcal{H}_2$ optimal control. In Section 3, modeling issues relevant to the CSTR $\mathcal{H}_2$ control problem is first addressed. Then the $\mathcal{H}_2$ controller with integral action is designed for CSTR model. The conclusions will be drawn in Section 4.

Slovak University of Technology in Bratislava, Radlinského 9, 81237 Bratislava, Slovakia, Tel: +421 2 524952 69, Fax: +421 2 52496469, e-mail: mikles@cvt.stuba.sk

II. $\mathcal{H}_2$ Optimal Control

The standard $\mathcal{H}_2$ optimal control problem consists of stabilizing a linear system in such a way that its transfer matrix attains a minimum norm in the Hardy space $\mathcal{H}_2$.

The plant is modeled by the transfer matrix

$$G(s) = \begin{bmatrix} G_{11}(s) & G_{12}(s) \\ G_{21}(s) & G_{22}(s) \end{bmatrix} \tag{1}$$

with

$$\begin{aligned} G_{11}(s) &= C_1(sI - A)^{-1}B_1, \\ G_{12}(s) &= C_1(sI - A)^{-1}B_2 + D_{12}, \\ G_{21}(s) &= C_2(sI - A)^{-1}B_1 + D_{21}, \\ G_{22}(s) &= C_2(sI - A)^{-1}B_2, \end{aligned}$$

where matrices $A, C_1, B_1, B_2, D_{12}, C_2, D_{21}$ are given by the input-state-output model of the plant

$$\begin{aligned} \dot{x}(t) &= Ax(t) + B_1v(t) + B_2u(t), \\ z(t) &= C_1x(t) + D_{11}v(t) + D_{12}u(t), \\ y(t) &= C_2x(t) + D_{21}v(t) + D_{22}u(t). \end{aligned} \tag{2}$$

It is assumed that: (A, B_1) stabilizable, (A, C_1) detectable, (A, B_2) stabilizable, (A, C_2) detectable

$$D_{12}^T C_1 = 0,\ B_1 D_{21}^T = 0,\ D_{12}^T D_{12} = I,\\ D_{21} D_{21}^T = I,\ D_{11} = D_{22} = 0.$$

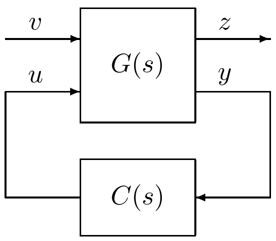

Fig. 1. Standard control configuration

Denoting $C(s)$ the transfer matrix of the controller, the control system transfer matrix between v and z for the feedback configuration shown in Fig. 1 becomes

$$\begin{aligned} H(s) &= G_{11}(s) \\ &\quad +G_{12}(s)\left[I - C(s)G_{22}(s)\right]^{-1} C(s)G_{21}(s). \end{aligned} \quad (3)$$

The standard $\mathcal{H}_2$ optimal control problem is given as follows [5]: Given a plant G, find a controller C that stabilizes the control system and minimizes $\mathcal{H}_2$ norm of H, defined as

$$\|H\| = \left(\frac{1}{2\pi j}\int tr\ H^T(-s)H(s)ds\right)^{1/2}, \quad (4)$$

where the integral is a contour integral up the imaginary axis and then around an infinite semicircle in the left half-plane.

In further derivations we will restrict ourselves to the singlevariable case. The $\mathcal{H}_2$ optimal control problem can be recast as a pole placement problem in which the dynamics induced by optimization is provided by two spectral factors $f(s)$ and $g(s)$.

The $\mathcal{H}_2$ optimal control law is given by

$$p(s)u = -q(s)y, \quad (5)$$

where the polynomials $p(s)$ and $q(s)$ satisfy the equation

$$a(s)p(s) + b(s)q(s) = f(s)g(s). \quad (6)$$

The polynomials $f(s)$ and $g(s)$ are defined by

$$N_L(s)N_L^T(-s) = f(-s)f(s), \quad (7)$$
$$N_R^T(-s)N_R(s) = g(s)g(-s), \quad (8)$$

where $a(s)$, $b(s)$, $N_L(s)$, and $N_R(s)$ are given by

$$\begin{aligned} C_2(sI - A)^{-1}B_2 &= \frac{b(s)}{a(s)}, \\ N_L(s) &= a(s)G_{21}(s), \\ N_R(s) &= G_{12}(s)a(s). \end{aligned}$$

If the closed-loop transfer function H is given by

$$H = \left[\begin{array}{c} W_1SV_1 \\ W_2UV_1 \end{array}\right], \quad (9)$$

where W_1, W_2, V_1 are shaping filters [6], then in the SISO case minimization of the 2-norm amounts to minimization of

$$\begin{aligned} \frac{1}{2\pi}\int_{-\infty}^{\infty} &\big(|W_1(j\omega)S(j\omega)V_1(j\omega)|^2 \\ &+|W_2(j\omega)U(j\omega)V_1(j\omega)|^2\big)d\omega. \end{aligned} \quad (10)$$

This is clearly the $\mathcal{H}_2$ version of the well-known mixed sensitivity problem of $\mathcal{H}_\infty$ optimization [4], [6].

The sensitivity function S determines the effect of the disturbance on the output of the control system. The complementary sensitivity T satisfies the identity $S + T = I$ and it is important for the closed-loop response, the effect of measurement noise and the amount of control effort. Shaping the input sensitivity function U is equivalent to shaping $T = G_{22}U$. It is possible to achieve the design goals by suitable choices of the functions V_1, W_1, and W_2.

III. CSTR $\mathcal{H}_2$ Control Problem

In this section, a nonlinear continuous stirred tank reactor (CSTR) problem will be considered. The $\mathcal{H}_2$ technique is applied here for control design. The application to the CSTR model will demonstrate usefulness of $\mathcal{H}_2$ control design to industrial problems.

A. Modeling of CSTR

We consider a CSTR by [7]. In the reactor an irreversible chemical reaction $A \rightarrow B$ take place. The rate of reaction is given as

$$r_A = kc_A, \quad k = k_0 e^{(-\frac{E}{R\vartheta})}. \quad (11)$$

Material and energy balances of this process are as follows [8]:

$$\begin{aligned} \frac{dx_1'}{dt} &= 1 - x_1' - \frac{V}{q}kx_1', && (12) \\ \frac{dx_2'}{dt} &= b - x_2' - \frac{F\alpha}{2\rho c_p}x_2' + \frac{F\alpha}{2\rho c_p}u' + \frac{V}{q\rho}kx_1', && (13) \\ k &= k_0 e^{\left(\frac{-gc_p}{c_{Av}H_r x_2'}\right)}, && (14) \end{aligned}$$

where

$$x_1' = \frac{c_A}{c_{Av}}, \qquad x_2' = \frac{c_p\vartheta}{c_{Av}H_r}, \qquad t = \frac{q}{V}t', \quad (15)$$
$$u' = \frac{c_p\vartheta_{ch}}{c_{Av}H_r}, \qquad b = \frac{c_p\vartheta_v}{c_{Av}H_r}, \qquad q = \frac{E}{R} \quad (16)$$

and

t'	time [min]
$c_A(t')$	concentration of A in reactor [mol m^{-3}]
$\vartheta(t')$	temperature of reactor [K]
$\vartheta_{ch}(t')$	temperature in cooling jacket [K]
$c_{Av}(t')$	concentration of A in feed stream [mol m^{-3}]
$\vartheta(t')$	temperature of feed stream [K]
V	volume of reactor [m^3]
q	volumetric feed rate [m^{3}min^{-1}]
k_0	reaction velocity constant [min^{-1}]
E	activation energy [kJ kmol^{-1}]
R	gas law constant [kJ kmol^{-1} K^{-1}]
c_p	specific heat of material in reactor [kJ kmol^{-1} K^{-1}]
H_r	heat of reaction [kJ kmol^{-1}]
ρ	density of material in reactor [kmol m^{-3}]
F	heat transfer area [m^2]
α	heat transfer coefficient [kJ min^{-1} m^{-2} K^{-1}]

Assumption required to write balances (12) and (13) are:

(a) The variables $k_0, E, c_p, H_r, \rho, \alpha$ are constant.

(b) Feed and product rates are identical and equal to q.

(c) The reactor is perfectly mixed.

The reactor described by (12) and (13) will be assumed as SISO system with one input u' and one output x_2'.

An important practical technique used in analyzing nonlinear systems is that of linearization. To apply the linear approximation technique, we first define new variables to shift the equilibrium state to the origin. Let $x_1'^s$ and $x_2'^s$ be the components of an equilibrium state of equations (12) and (13). Then

$$\begin{aligned} 0 &= 1 - x_1'^s - f_1'(x_1'^s, x_2'^s), &(17)\\ 0 &= b - x_2'^s - f_2'(x_2'^s) + f_3'(u'^s) + \frac{1}{\rho} f_1'(x_1'^s, x_2'^s), &(18)\end{aligned}$$

where

$$\begin{aligned} f_1'(x_1', x_2') &= \frac{V}{q} x_1' k_0 e^{\left(\frac{-gc_p}{c_{A_v} H_r x_2'}\right)}, &(19)\\ f_2'(x_2') &= \frac{F\alpha}{q\rho c_p} x_2', &(20)\\ f_3'(u') &= \frac{F\alpha}{q\rho c_p} u'. &(21)\end{aligned}$$

We define:

$$x_1 = x_1' - x_1'^s, \quad x_2 = x_2' - x_2'^s, \quad u = u' - u'^s,$$

$$\begin{aligned} f_1(x_1, x_2) &= f_1'(x_1' + x_1'^s, x_2' + x_2'^s) - f_1'(x_1'^s, x_2'^s),\\ f_2(x_2) &= f_2'(x_2' + x_2'^s) - f_2'(x_2'^s),\\ f_3(u) &= f_3'(u' + u'^s) - f_3'(u'^s),\end{aligned}$$

then equations (12) and (13) reduce to

$$\begin{aligned} \frac{dx_1}{dt} &= -x_1 - f_1(x_1, x_2), &(22)\\ \frac{dx_2}{dt} &= -x_2 - f_2(x_2) + f_3(u) + \frac{1}{\rho} f_1(x_1, x_2), &(23)\end{aligned}$$

with $f_1(0,0) = 0$, $f_2(0) = 0$, and $f_3(0) = 0$.

The linearized model for CSTR is:

$$\begin{aligned} \frac{dx}{dt} &= Ax + B_2 u, &(24)\\ x &= (x_1, x_2)^T,\\ A &= \begin{pmatrix} a_{11p} & a_{12p}\\ a_{21p} & a_{22p}\end{pmatrix}, \quad B_2 = \begin{pmatrix} 0\\ b_{21p}\end{pmatrix},\\ a_{11p} &= -1 - \frac{\partial f_1}{\partial x_1}(0,0),\\ a_{12p} &= -\frac{\partial f_1}{\partial x_2}(0,0),\\ a_{21p} &= \frac{1}{\rho}\frac{\partial f_1}{\partial x_1}(0,0),\\ a_{22p} &= -1 - \frac{\partial f_2}{\partial x_2}(0) + \frac{1}{\rho}\frac{\partial f_1}{\partial x_2}(0,0),\\ b_{21p} &= \frac{\partial f_3}{\partial u}(0).\end{aligned}$$

The non-linearity in equations (22) and (23) is solely a function of the state variables and therefore would be equivalent to uncertainty in state-space A matrix. The physics of the problem already improve same useful bounds on the state variables. For the purposes of $\mathcal{H}_2$ version of the mixed sensitivity problem of $\mathcal{H}_\infty$ optimization is useful impose bounds on the state variables which define an operating window in the phase plane.

B. $\mathcal{H}_2$ optimal controller

The system matrices for the CSTR described by equation (24) in standard state–space form are given by

$$\left[\begin{array}{ccc} A & B_1 & B_2\\ C_1 & D_{11} & D_{12}\\ C_2 & D_{21} & D_{22}\end{array}\right] = \left[\begin{array}{cc|ccc|c} a_{11p} & a_{12p} & b_{111} & 0 & 0 & 0\\ a_{21p} & a_{22p} & 0 & b_{122} & 0 & b_{21p}\\ \hline c_{111} & 0 & 0 & 0 & 0 & 0\\ 0 & c_{122} & 0 & 0 & 0 & 0\\ c_{131} & c_{132} & 0 & 0 & 0 & 1\\ \hline 0 & 1 & 0 & 0 & 1 & 0\end{array}\right]. \qquad (25)$$

v comprises the driving signals for the shaping filters for disturbances and measurement noise. b_{111}, b_{122}, c_{111}, c_{122}, c_{131}, and c_{132} can be design parameters.

The standard $\mathcal{H}_2$ design procedure does not give a controller with integral action. There are several ways to introduce it. One approach is to augment the plant with an integrator before starting the design and then to use this integrator as a part of the final controller. The transfer function of the augmented plant can have the form

$$G_{aug1}(s) = \left[\begin{array}{cc|c} 1 & 0 & B_I\\ B_2 & A & B_2\\ \hline 0 & C_2 & 0\end{array}\right] \qquad (26)$$

or

$$G_{aug2}(s) = \left[\begin{array}{cc|c} A & 0 & B_2\\ B_I C_2 & 0 & 0\\ \hline C_2 & 1 & 0\end{array}\right], \qquad (27)$$

where the integral part of the controller is given by the transfer function

$$G_I(s) = \left[\begin{array}{c|c} 0 & B_I \\ \hline 1 & 1 \end{array}\right] , \quad B_I = \beta. \tag{28}$$

Now, if the resulting $\mathcal{H}_2$ controller stabilizes the plant and makes the 2 norm between v_3 and z_3 finite, then the controller must have a pole at $s = 0$ which is the zero of the sensitivity function.

The augmented system matrices for the CSTR described by equation (24) and G_{aug1} in standard state–space form are given by

$$\begin{bmatrix} A_a & B_{1a} & B_{2a} \\ C_{1a} & D_{11a} & D_{12a} \\ C_{2a} & D_{21a} & D_{22a} \end{bmatrix} =$$

$$\left[\begin{array}{ccc|cccc|c} 0 & 0 & 0 & b_{111} & 0 & 0 & 0 & \beta \\ 0 & a_{11p} & a_{12p} & 0 & b_{122} & 0 & 0 & 0 \\ b_{21p} & a_{21p} & a_{22p} & 0 & 0 & b_{133} & 0 & b_{21p} \\ \hline c_{111} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c_{122} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & c_{133} & 0 & 0 & 0 & 0 & 0 \\ c_{141} & c_{142} & c_{143} & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right] . \tag{29}$$

The entries of B_{1a} and C_{1a} matrices and β are design parameters.

Note 1: The standard state-space form (29) is the basis for next loop shaping design procedure.

□

Relevant constants of the CSTR for the case study are given as follows:

$$\begin{array}{cccc} c_{Av} = 0.88, & \vartheta = 370, & V = 1.8, & q = 0.25, \\ k_0 = 1\text{x}10^{10}, & g = 11078, & c_p = 4.05, & H_r = 149280, \\ \rho = 970, & F = 5.04, & \alpha = 130, & i_m = 5\text{x}10^{-13}, \end{array}$$

where i_m is intensity of measurement noise.

If $b_{111} = 0.5$, $b_{122} = 0.6$, $b_{133} = 0.7$, $c_{111} = 100$, $c_{122} = 100$, $c_{133} = 50$, $c_{141} = 5$, $c_{142} = 6$, $c_{143} = 7$, and $\beta = 0.5$ then the transfer function of the $\mathcal{H}_2$ optimal controller is given by

$$C(s) = \frac{(53.68s^2 + 139.5s + 85.65)(s + \beta)}{s^4 + 63.38s^3 + 132.2s^2 + 69.41s} . \tag{30}$$

The corresponding MATLAB script for controller design macros of Polynomial Toolbox 2.0 is given

```
A=Aa; B2=B2a; B1=B1a;
C1=C1a; C2=C2a;
D12=D12a; D21=D21a;

[BLS,AL]=ss2lmf(A,eye(3),C2);
[BRS,AR]=ss2rmf(A,B2,eye(3));

f=spf((BLS*B1+AL*D21)*(BLS*B1+AL*D21)');
g=spf((C1*BRS+D12*AR)'*(C1*BRS+D12*AR));
```

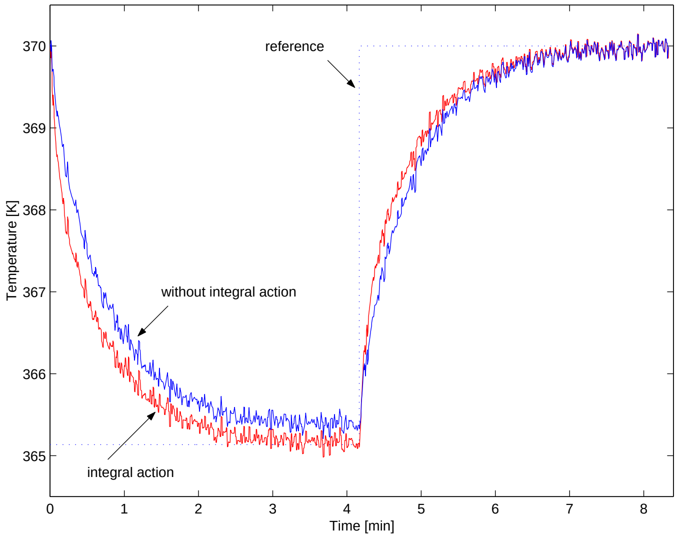

Fig. 2. Responses of output temperature

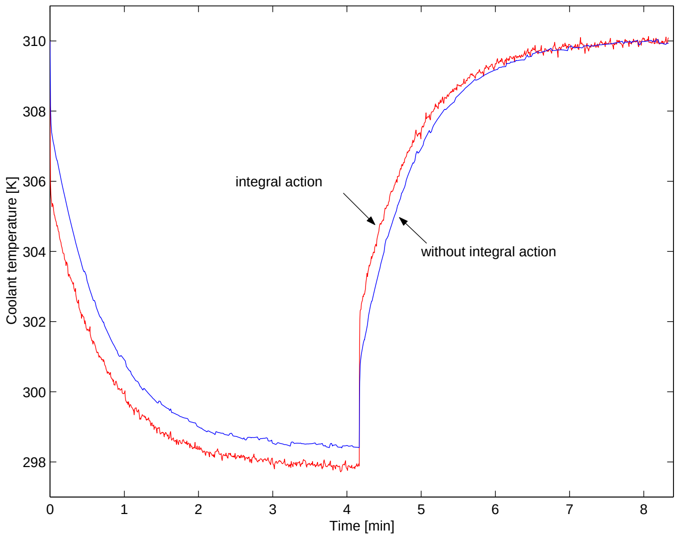

Fig. 3. Responses of coolant temperature

```
BL=BLS*B2;
BR=C2*BRS;
[XP,YP]=axbyc(AR,BR,f*g,'min');
YP=YP/lcoef(XP),XP=XP/lcoef(XP);

C=-tf(YP,XP)*tf(s+beta,s);
```

In Figs. 2, 3, and 4 reference tracking properties are demonstrated.

IV. Conclusion

The simulation results support the applicability of $\mathcal{H}_2$ control technique to industrial problems. The paper presents the polynomial approach to $\mathcal{H}_2$ optimization problem applied to a chemical reactor. The $\mathcal{H}_2$ optimal controller with integral action has been presented. The appli-

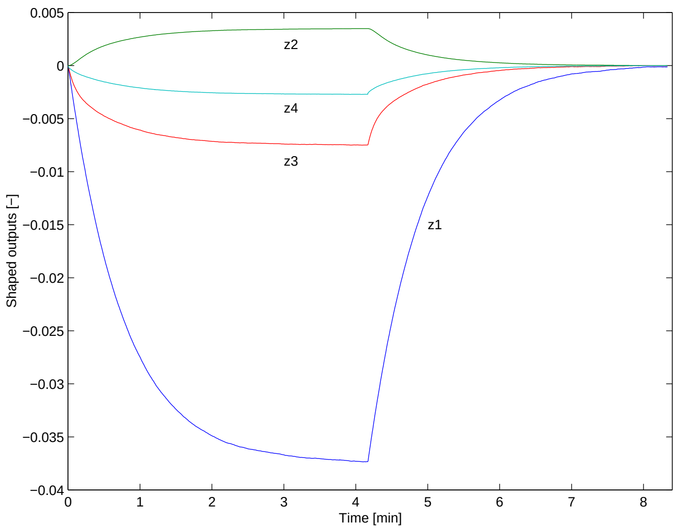

Fig. 4. Responses of shaped outputs

cation of the Matlab Polynomial Toolbox makes the design of the $\mathcal{H}_2$ controller very simple.

The designed optimal controller with integral action and loop shaping was developed and used for control of a laboratory chemical reactor.

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