An Iterative Identification and Control Design of a Chemical Reactor

†Š. KOŽKA and J. MIKLEŠ

Department of Information Engineering and Process Control, Faculty of Chemical and Food Technology, Slovak University of Technology, SK-812 37 Bratislava
e-mail: mikles@cvt.stuba.sk

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This contribution deals with temperature stabilization of a continuous stirred tank reactor. Here, the modified iterative scheme of system identification and control design is combined. Based on identification, the feedback controller is designed, which stabilizes the reactor at an arbitrary set point in spite of uncertainties in the kinetics. The iterative identification is based on the Youla—Kucera parametrization. The main advantage of the used algorithm is that it is not necessary to apply the reduction method during the identification as in the standard identification realized *via* mentioned parametrization.

The literature contains a large number of papers that discuss the design and control of chemical reactors. Textbooks such as [1] and [2] present the fundamentals, but the emphasis is primarily on steady-state aspects. These texts cover some topics in dynamics, but most of the discussion is about stability and multiple steady states.

In the last ten years, there has been a great deal of activity in the nonlinear feedback control and stabilization of chemical reactors. Typical references among others are [3—6]. The engineering motivation relies on the fact that the reactor operation in states corresponds to an optimal process performance (like, for instance, an optimum tradeoff between yield and productivity). These states can lie near or at unstable steady state.

Feedback control of chemical reactors is a problem, which is made difficult by the inherent nonlinear nature of the involved mechanism. One of the particular control problems, which were most commonly investigated, is the temperature regulation of an exothermic irreversible reaction in a cooled continuously stirred tank reactor (CSTR). The reaction and the reactor considered in this paper are quite simple.

Here, a controller that guarantees temperature stabilization in spite of strong uncertainties in the kinetic function with respect to the temperature is proposed. Our control design is based on parametrization of identified linear model of laboratory reactor. The "classical" principles of identification can be found in textbook as [7]. Of special interest is the situation when the data to be used have been collected under closed-loop operation.

A collection of recently developed controller design methods founded on iterations of plant model identification and controller design is presented in [8] and [9]. The main problem studied in these two survey papers is how to obtain the optimal controller from model, which optimally resembles the system in closed loop.

In this paper the iterative identification, based on the Youla—Kucera parametrization, for control design is used. The quality of each candidate estimated model depends on its own controller and *vice versa*. The major drawback of standard iterative scheme, based on the Youla—Kucera parametrization, is that the order of identified model is not simply tunable due to the required reparametrization, *i.e.* application of a reduction technique. The algorithm presented in this contribution eliminated this drawback. Our modified iterative scheme is composed of an optimal control design method and a prediction error identification technique.

SYSTEM DESCRIPTION AND PROBLEM FORMULATION

System Configuration

The reactor (Fig. 1, liquid volume approximately 0.95 dm^3) consists of a glass tube closed by two gastight stainless steel lids. The glass coil *9* with heat transfer area 0.065 m^2 represents the cooling system of reactor. Water has been used as a coolant. Two peristaltic pumps *1*, *2* meter both reactants (H_2O_2 and $K_2Cr_2O_7$) and feed reactor near the mixer *5*. The reaction products are taken away by an overflow *10*, which also provides constant liquid volume. Products are divided into gas *7* and liquid phases *8*. The ther-

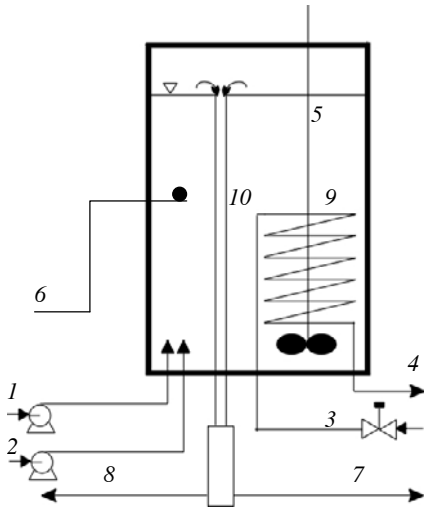

Fig. 1. Laboratory reactor system.

mometer *6* protected from corrosion by polyethylene shield measures the temperature in the reactor. The temperatures of inlet *3* and outlet coolant *4* are also measured. The pneumatic valve continuously controls the coolant feed. In the reactor an exothermic reaction, dissociation of hydrogen peroxide,

$$2\mathrm{H_2O_2} \xrightarrow{\mathrm{K_2Cr_2O_7}} 2\mathrm{H_2O} + \mathrm{O_2}$$

takes place. The following material and energy balances give the mathematical model of CSTR

$$\frac{\mathrm{d}c_\mathrm{A}}{\mathrm{d}t} = \frac{1}{V}(q_\mathrm{A}c_\mathrm{AV} - (q_\mathrm{A}+q_\mathrm{B})c_\mathrm{A}) - 2\nu(c_\mathrm{A}, c_\mathrm{B}, \vartheta) \quad (1)$$

$$\frac{\mathrm{d}\vartheta}{\mathrm{d}t} = \frac{1}{C_p\rho}(-\Delta H)2\nu(c_\mathrm{A}, c_\mathrm{B}, \vartheta) + \frac{q_\mathrm{A}+q_\mathrm{B}}{V}(\vartheta_\mathrm{V} - \vartheta) - \\ - \frac{A\alpha}{C_pV\rho}(\vartheta - \vartheta_\mathrm{CH}) - \frac{k_\mathrm{s}A\alpha}{C_pV\rho}(\vartheta - \vartheta_\mathrm{out}) \quad (2)$$

$$\frac{\mathrm{d}\vartheta_\mathrm{CH}}{\mathrm{d}t} = \frac{q_\mathrm{CH}}{V_\mathrm{CH}}(\vartheta_\mathrm{CHV} - \vartheta_\mathrm{CH}) + \\ + \frac{A\alpha}{C_{p_\mathrm{CH}}V_\mathrm{CH}\rho_\mathrm{CH}}(\vartheta - \vartheta_\mathrm{CH}) \quad (3)$$

where

$$\nu(c_\mathrm{A}, c_\mathrm{B}, \vartheta) = kc_\mathrm{A}^{z_1}c_\mathrm{B}^{z_2}\mathrm{e}^{\frac{E(\vartheta-\vartheta_0)}{R\vartheta\vartheta_0}}$$

and

$$c_\mathrm{B} = \frac{c_\mathrm{BV}q_\mathrm{B}}{q_\mathrm{A}+q_\mathrm{B}}$$

The detailed information about this reactor can be found in [10].

Problem Formulation

Consider now that the task is to identify the simple model of plant G_0, shown in Fig. 2, that is stabilized

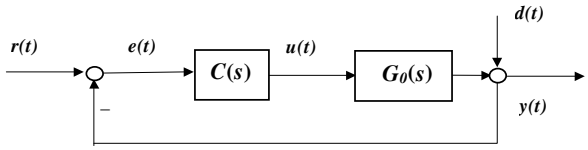

Fig. 2. Closed-loop configuration. e – control error, - negative feedback.

by the controller C. Here, $u(t)$ and $y(t)$ are measurable input and output signals, respectively. The system with negative feedback is driven by the reference signal (set-point) $r(t)$ and additive output noise $d(t)$.

The procedure presented here is based on the idea that in each step a control-relevant model is estimated and subsequently, if the controller performance is not satisfactory, a new controller is designed. It is assumed that the initial controller, the controller that is used in the first estimation, is available which stabilizes the laboratory reactor but otherwise shows unsatisfactory performance (*e.g.* excessive overshoot, rise-time not small enough, *etc.*). The goal is to systematically improve the controller performances.

In our case, the continuous stirred tank reactor, shown in Fig. 1, represents the plant. The measurable input signal $u(t)$ is given by the rate of coolant q_CH and $y(t)$ is equal to temperature of reactant mixture ϑ. The notation and the problem setup of [11] is used through this paper.

Assumption 1
Assume that the controller

$$C(s) = \frac{Q(s)}{P(s)} \quad (4)$$

with coprime factors $P(s) = \dfrac{p(s)}{m_2(s)}$ and $Q(s) = \dfrac{q(s)}{m_2(s)}$ from R_ps is known and stabilizes the plant $G_0(s)$

$$G_0(s) = \frac{B_0(s)}{A_0(s)} \quad (5)$$

with coprime elements $A_0(s) = \dfrac{a_0(s)}{m_1(s)}$, $B_0(s) = \dfrac{b_0(s)}{m_1(s)}$ from R_ps, and consider the nominal (auxiliary) model $G_\mathrm{N}(s)$ that is stabilized by C.

$$G_\mathrm{N}(s) = \frac{B_\mathrm{N}(s)}{A_\mathrm{N}(s)} \quad (6)$$

where $A_\mathrm{N}(s) = \dfrac{a_\mathrm{N}(s)}{m_1(s)}$ and $B_\mathrm{N}(s) = \dfrac{b_\mathrm{N}(s)}{m_1(s)}$ are particular solutions of the following Bezout identity

$$A_\mathrm{N}P + B_\mathrm{N}Q = 1 \quad (7)$$

In eqns (*4—6*) the parameters $a_0(s)$, $b_0(s)$, $a_N(s)$, $b_N(s)$, $p(s)$, $q(s)$, $m_1(s)$, $m_2(s)$ are polynomials and s is operator of a Laplace transformation. R_{ps} denotes the set of stable proper rational functions. *Assumption 1* expresses both the fact that the factors A_N, B_N, P, and Q are coprime and that the feedback loop formed by the nominal model G_N and controller C is internally stable [12]. If the actual controller C is a stabilizing controller for the plant G_0 (see *Assumption 1*), there exists a unit U from R_{ps}, such that

$$A_0P + B_0Q = U = \frac{m_3m_4}{m_1m_2} \tag{8}$$

where $m_3m_4 = a_0p + b_0q$.

ITERATIVE IDENTIFICATION

Identification Based on the Youla—Kucera Parametrization

In this section we will present the identification method that is used for identification of a simple model of unknown plant in closed-loop configuration (see Fig. 2). *Hansen* and *Franklin* [13] introduce the basic idea of the iterative identification based on a dual Youla—Kucera parametrization. It was further elaborated in [14] and modified for approximate identification in [15].

Theorem 1 [13]

Let *Assumption 1* hold. Then the set of all possible plant models for which the closed-loop system shown in Fig. 2 remains internally stable is characterized as

$$G_0 = \frac{B_N + PR}{A_N - QR} \tag{9}$$

where the Youla—Kucera parameter $R(s) = \dfrac{n_R(s)}{d_R(s)}$ is a stable proper rational function. Here $n_R(s)$ and $d_R(s)$ are polynomials of $R(s)$.

Theorem 1 represents the standard parametrization of the class of all plants that are stabilized by the actual controller $C(s)$. The idea of this approach is to identify the parameter $R(s)$ and then the transfer function $G_0(s)$ is computed from eqn (*9*). For identification of $R(s)$ auxiliary signals $z(t)$ and $x(t)$ are utilized [15].

$$\begin{aligned} z(t) &= A_Ny(t) - B_Nu(t) \\ x(t) &= Qy(t) - Pu(t) \end{aligned} \tag{10}$$

With respect to the mentioned auxiliary signals, the parameter $R(s)$ has the following form

$$z(t) = Rx(t) + d(t) \tag{11}$$

This method is attractive, because identified plant models are guaranteed to be stabilized by the present controller [15]. On the other hand, during the identification the complexity of identified model increases at the end of each iteration, because the order of identified plant increases through the estimated Youla—Kucera parameter [9]. This fact represents a serious drawback of this approach if the controller with the fixed structure is used. In that case, it is necessary to identify also the model with fixed structure. This is the reason why the model reduction algorithm must be used. If the mentioned reduction is utilized, then the structure of identified model is not changed at the end of each iteration. Our idea here is to modify the algorithm presented in [15], based on eqns (*9—11*) in such a way that the model reduction step will be eliminated and structure of identified model will be fixed.

Modified Iterative Identification

The main idea of this modification is that the polynomial n_R (numerator of $R(s)$) is identified rather than the parameter $R(s)$. This polynomial is estimated through the signals $x_F(t)$ and $z_F(t)$ which can be calculated by filtering the measured data $y(t)$ and $u(t)$ with filters F_1 and F_2 [11].

$$\begin{aligned} z_F(t) &= F_1(A_Ny(t) - B_Nu(t)) \\ x_F(t) &= F_2(Pu(t) + Qy(t)) \\ F_1 &= \frac{m_3m_4}{m_2m_2} \\ F_2 &= \frac{1}{m_1m_2} \end{aligned} \tag{12}$$

Since it is not necessary to identify the denominator of the Youla—Kucera parameter and with respect to the filtered auxiliary signals the relation (*11*) can be expressed as follows [11]

$$z_F(t) = n_Rx_F(t) + d(t) \tag{13}$$

The plant model $\hat{G}_0 = \hat{G}_0(n_R)$ can be calculated using the relation [11]

$$a_N\hat{b}_0 - b_N\hat{a}_0 = n_R = n_{R1}s + n_{R0} \tag{14}$$

where $\hat{a}_0$, $\hat{b}_0$ are polynomials of the plant model $\hat{G}_0 = \dfrac{\hat{b}_0(s)}{\hat{a}_0(s)}$ and n_{R1}, n_{R0} are estimated coefficiens of polynomial n_R. The relation (*14*) shows that if the right hand of this equation is the polynomial of constant order and a_N, b_N are polynomials with constant order, then computed polynomials $\hat{a}_0$, $\hat{b}_0$ of the plant model $\hat{G}_0 = \dfrac{\hat{b}_0(s)}{\hat{a}_0(s)}$ have also constant order. It means that at the end of each iteration, the computed plant

model has fixed structure and it is not necessary to use reduction algorithm as in standard identification based on the Youla—Kucera parametrization. Moreover, eqn (*14*) shows that if $\hat{a}_0$, $\hat{b}_0$ are the same as a_N, b_N, then the right hand of this equation must be a zero polynomial.

Consider that we have collected a data set $\{y(t), u(t)\}$ of the length N (see Fig. 2). Then the i-th iteration of the modified iterative algorithm consists of the following steps:

Step 1: Based on known C_{i-1}, $G_{N,i-1}$, and $(m_3m_4)_{i-1}$ construct the stable filters $F_{1,i}$, $F_{2,i}$ and filtered auxiliary signals $z_F(t)$, $x_F(t)$ *via* eqn (*12*).

Step 2: Use the filtered auxiliary signals in the least-squares identification algorithm, considering $z_F(t)$ as output signal and $x_F(t)$ as input signal, and identify the polynomial $n_{R,i}$.

Step 3: Compute the new transfer function of the identified model $\hat{G}_{0,i} = \dfrac{\hat{b}_{0,i}(s)}{\hat{a}_{0,i}(s)}$ from eqn (*14*).

Step 4: Construct the polynomial $(m_3m_4)_i = \hat{a}_{0,i}p_{i-1} + \hat{b}_{0,i}q_{i-1}$.

Step 5: Specify or calculate $(m_1m_2)_i$ and use relations $a_{N,i}(s) = \hat{a}_{0,i}(s), b_{N,i}(s) = \hat{b}_{0,i}(s)$.

Step 6: Design new controller C_i according to eqn (*7*).

Step 7: Increase i, $i = i + 1$, and go to Step 1.

The iterations are finished when the coefficients of identified polynomial $n_{R,i}$ reach the values close to zero. Then the final controller (Step 6 of the last iteration) is applied to the true plant and, if it is necessary, the new collection of data set $\{y(t), u(t)\}$ together with new iterative identification is realized.

EXPERIMENTAL

The results from identification of laboratory continuous stirred tank reactor are presented. The estimation of plant model was realized *via* modified iterative identification proposed above. The total number of estimations (collection of data sets) was three. Each estimation consisted of 10 iterations.

First Estimation

For the first estimation the process was controlled using an a priori designed LQ controller *via* linearization technique of nonlinear model described by eqns (*1—3*). Detailed information about controller design can be found in [16]. This controller was tuned for the set-point $r = 303.15$ K (30 °C). The goal of the iterative design for this case is to compute the controller with zero overshoot.

The process was excited by changing of set-point from $r = 303.15$ K (30 °C) to $r = 306.15$ K (33 °C). For control-relevant system identification to obtain polynomial n_R, the modified least-squares (LS) algorithm

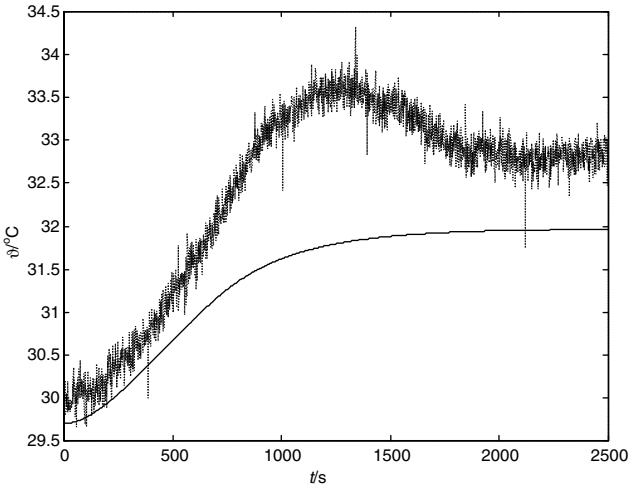

Fig. 3. Output responses to set-point change – the first estimation, experimental (dotted), model (solid).

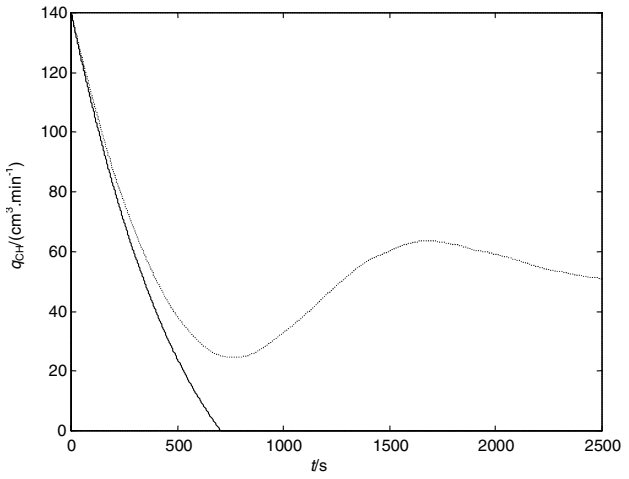

Fig. 4. Input responses to set-point change – the first estimation, experimental (dotted), model (solid).

was applied (see [17] and [18]). The model parameters were recursively estimated in discrete time intervals [19].

In the case of the first estimation the simulated closed loop was given by controller C and nominal model (obtained by linearization of nonlinear model) G_N. The same controller was applied on the laboratory reactor. Comparison of both closed loops is shown in Figs. 3 and 4, respectively.

Based on the presented responses we can say that the simulated closed loop does not fit the experimental one. Moreover, the coolant feed rate (simulated closed loop) reached the low saturation limit during the simulation (see Fig. 4). The range for coolant feed rate was between 0 and 2.33 cm^3 s^{-1}. Fig. 3 shows that the designed controller applied to the laboratory reactor has a poor performance. The overshoot was 16.6 % and the time of stabilization was longer than 2000 s.

Second Estimation

The collected experimental data, controller C, and nominal model G_{N} from the previous step were used in the second estimation. In any iteration the polynomial n_{R} was estimated and using eqn (*10*) the new plant model was computed. Based on the $\hat{G}_0 = \dfrac{\hat{b}_0(s)}{\hat{a}_0(s)}$ the new controller C was designed. The iterative algorithm was stopped when the identified coefficients $n_{\mathrm{R1}}, n_{\mathrm{R0}}$ were close to zero. The resulted controller was then applied either to the laboratory reactor or to the computed model. The new comparison of both closed loops is shown in Figs. 5 and 6.

The results shown in Figs. 5 and 6 demonstrate that the properties of designed controller were improved. The overshoot was eliminated. Moreover, the static and dynamic properties of simulated closed loop well corresponded with the real plant. The time of stabilization of laboratory reactor was still about 2000 s.

Third Estimation

The process was identified again with the aim to short the time of stabilization of the reactor and to minimize the differences between compared closed loops. Again the collected experimental data and controller from the previous step were used. In this case, the identified plant model from the second estimation replaced the nominal model G_{N}. The iterative algorithm then provided the new estimation of the plant model that was used as a basis for control design step. The new controller was again applied either to the laboratory reactor or to just estimated plant model. Comparison of both closed loops is shown in the following figures.

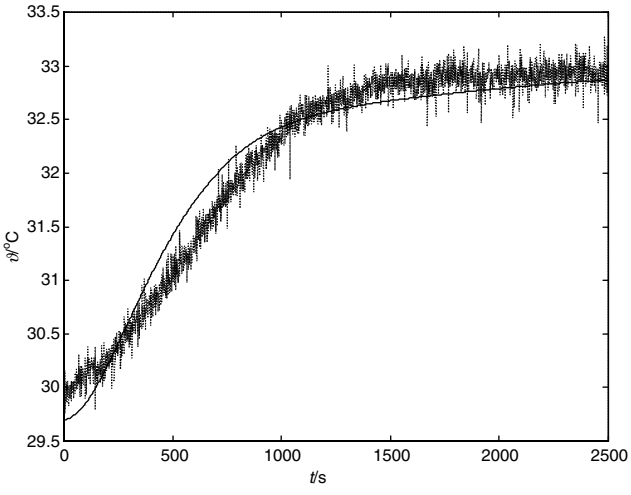

Fig. 5. Output responses to set-point change – the second estimation, experimental (dotted), model (solid).

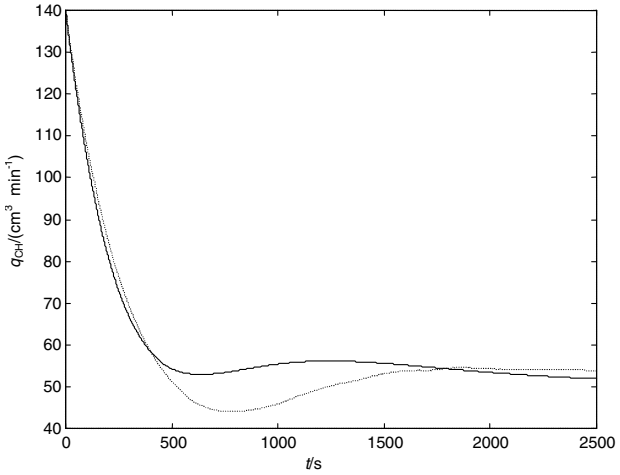

Fig. 6. Input responses to set-point change – the second estimation, experimental (dotted), model (solid).

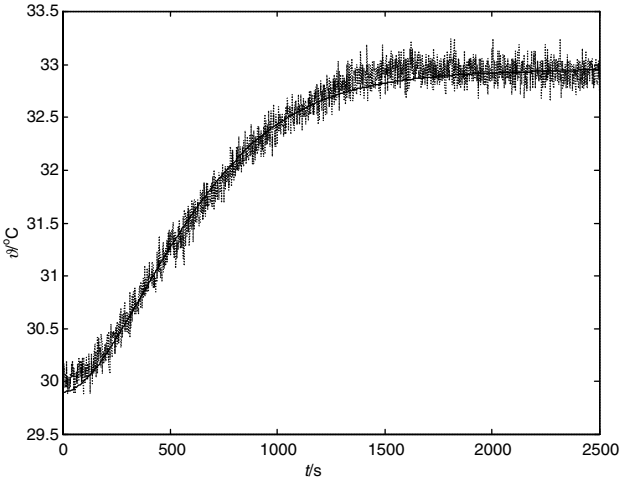

Fig. 7. Output responses to set-point change – the third estimation, experimental (dotted), model (solid).

Figs. 7 and 8 show that the measured and predicted responses are very close. It can thus be concluded that the model obtained from closed-loop data is sufficiently accurate for the used set-point change. Note that good approximation for other set-point changes is of less importance. The time of stabilization of laboratory reactor was about 1600 s.

CONCLUSION

An iterative scheme for closed-loop identification was applied to the identification and control of laboratory scale continuous stirred tank reactor. The modified iterative scheme of system identification, based on the Youla—Kucera parametrization, and control design were combined. It was demonstrated that the estimated models despite process nonlinearities and controller constraints, are control-relevant and that

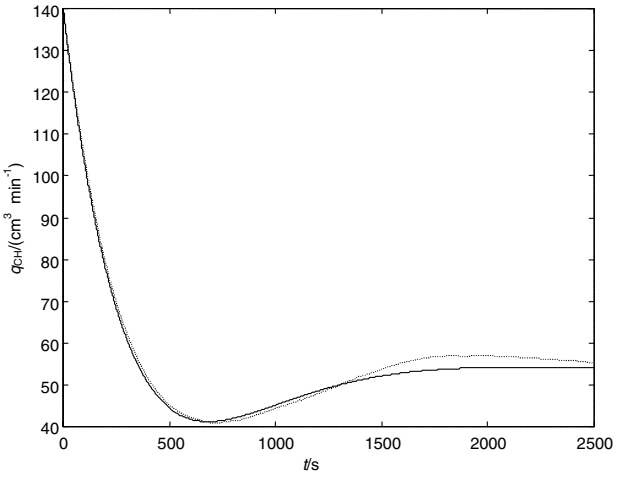

Fig. 8. Input responses to set-point change – the third estimation, experimental (dotted), model (solid).

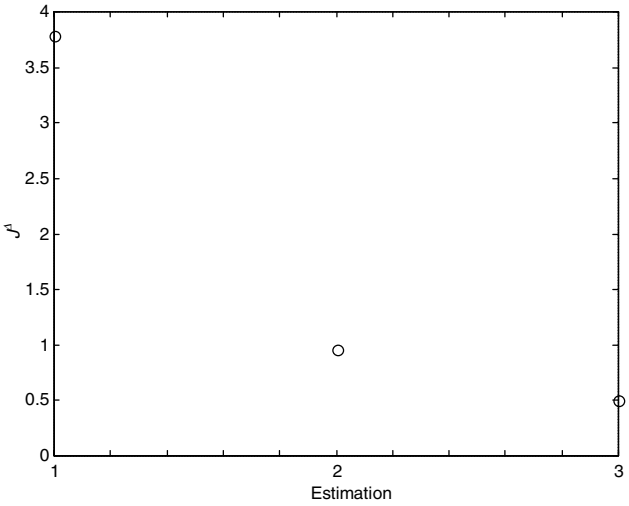

Fig. 9. Performance error.

controllers can systematically be improved during the estimations. In the identification step a controller-relevant process model is obtained by the identification of the polynomial $n_{\mathrm{R}}(s)$ using time-domain data. The main advantage of the modified algorithm is that it is not necessary to use the reduction algorithm as in the standard approach based on the mentioned parametrization.

In effort to measure the differences between simulated and experimental closed loops the following equation was computed [15]

$$J^{\Delta} = \int_0^{\infty} [\mu(y(t) - y_{\mathrm{c}}(t))^2 + \varphi(\dot{u}(t) - u_{\mathrm{c}}(t))^2]\mathrm{d}t \quad (15)$$

Here, $y_{\mathrm{c}}(t)$, $u_{\mathrm{c}}(t)$ represent the output and input signal of simulated closed loop and μ, φ are weighting coefficients used in controller design step. J^{Δ} expresses the performance error that results from applying controller C designed for plant model $\hat{G}_0$, to the actual plant G_0. This error will be small if the actual loop and simulated loop are "close to one another in the appropriate sense". Fig. 9 shows that in this case the computed performance error systematically decreased.

It should be noted that the used iterative procedure requires the acquisition of additional data as each new controller is generated. In industrial applications this will usually be feasible because the data are recorded with the plant in closed loop, which is usually more easily tolerated by plant operators than collecting data with the controller in manual mode.

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SYMBOLS

c_{A}	H_2O_2 concentration	mol m^{-3}
c_{AV}	inlet H_2O_2 concentration	mol m^{-3}
c_{B}	$K_2Cr_2O_7$ concentration	mol m^{-3}
c_{BV}	inlet $K_2Cr_2O_7$ concentration	mol m^{-3}
q_{A}	H_2O_2 feed rate	m^3 s^{-1}
q_{B}	$K_2Cr_2O_7$ feed rate	m^3 s^{-1}
q_{CH}	coolant feed rate	m^3 s^{-1}
ν	specific reaction rate	mol m^{-3} s^{-1}
V	liquid volume of reactor	m^3
ρ_{CH}	density of the coolant	kg m^{-3}
C_{P}	heat capacity of the reactor contents	J kg^{-1} K^{-1}
C_{PCH}	heat capacity of the coolant	J kg^{-1} K^{-1}
ϑ	reactor temperature	K
ϑ_{CH}	outlet temperature of the coolant	K
ϑ_{CHV}	inlet temperature of the coolant	K
ϑ_{OUT}	outer temperature	K
A	heat transfer area	m^2
α	heat transfer coefficient	W m^{-2} K^{-1}
k	reaction rate constant	s^{-1}
z_1, z_2	the orders of the reaction	1
$-\Delta H$	heat of the reaction	J mol^{-1}
$u(t)$	input signal	m^3 s^{-1}
$y(t)$	output signal	K
$u_{\mathrm{c}}(t)$	simulated input signal	m^3 s^{-1}
$y_{\mathrm{c}}(t)$	simulated output signal	K
$r(t)$	reference signal	K
$d(t)$	noise signal	
$z(t), x(t)$	auxiliary signals	
$z_{\mathrm{F}}(t), x_{\mathrm{F}}(t)$	filtered auxiliary signals	
t	time	s
s	operator of the Laplace transformation	
$G_0(s)$	transfer function of laboratory reactor	
$\hat{G}_0(s)$	transfer function of plant model	
$G_{\mathrm{N}}(s)$	transfer function of nominal model	
$C(s)$	transfer function of controller	

$R(s)$ transfer function of the Youla—Kucera parameter
$F_1(s), F_2(s)$ transfer function of filters
$A_0(s), B_0(s)$ coprime factors of $G_0(s)$
$A_N(s), B_N(s)$ coprime factors of $G_N(s)$
$Q(s), P(s)$ coprime factors of $C(s)$
$a_0(s), b_0(s)$ polynomials of $G_0(s)$
$\hat{a}_0(s), \hat{b}_0(s)$ polynomials of $\hat{G}_0(s)$
$a_N(s), b_N(s)$ polynomials of $G_N(s)$
$p(s), q(s)$ polynomials of $C(s)$
$n_R(s), d_R(s)$ polynomials of $R(s)$
$m_1(s), m_2(s)$ poles of simulated closed loop
$m_3(s), m_4(s)$ poles of actual closed loop
R_{ps} stable proper rational functions
U unit from R_{ps}
φ, μ weighting factors

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