A ROBUST AND ADAPTIVE APPROACH TO CONTROL OF A CONTINUOUS STIRRED TANK REACTOR WITH JACKET COOLING

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KEYWORDS

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ABSTRACT

Continuous Stirred Tank Reactors (CSTR) are one of the main technological plants used in chemical and biochemical industry. These systems are quite complex with many nonlinearities and the conventional linear control with fixed parameters can be questionable or sometimes unacceptable. The solution should be found in so-called "non-traditional" control approaches like adaptive, robust, fuzzy, or artificial intelligent methods. One way is the utilization of self-tuning adaptive schemes, but computations may be quite difficult, clumsy and time-consuming. This paper brings an alternative principle called a robust approach and the comparison of the robust and adaptive control responses. Robust control considers a CSTR model as a linear system with parametric uncertainty, which covers a family of all feasible plants. Then several controllers with fix parameters are designed so that for all possible plants, the acceptable control behavior is obtained. The two-degree-of-freedom (2DOF) structure for the control law was chosen. Both robust and adaptive control is applied to an original nonlinear model of a CSTR. All calculations and simulations of mathematical models and control responses were performed in the Matlab and Simulink environment.

INTRODUCTION

The plants in technological processes and especially in chemical and biochemical industry usually have nonlinear behavior that causes difficulties in the control of such processes. Another unpleasant feature can be found in the complexity of such processes with a lot of variables and properties that result in difficult mathematical descriptions. This negative property should be overcome with the linearization of nonlinear models that introduces simplifications that reduces the intricacy of the system. On the other hand, this simplification can result in inaccurate descriptions of the system. The utilization of adaptive (e.g. self-tuning) schemes brings more difficult, clumsy and timeconsuming computations (Åström and Wittenmark

1989). The control design using a hybrid adaptive control principle was used in (Vojtesek et al. 2017) where the originally nonlinear system was represented by an external linear model with recursively identified parameters and the pole-placement method adjustment principle was applied. A practically favored approach to overcome the loss of the model accuracy, compensated by its structure simplicity, consists in the utilization of a model with uncertainty. This idea allows working with the linear time-invariant low order mathematical models also for the case of real systems with complex dynamics or nonlinear behavior. There are several ways how to incorporate the uncertainty into the mathematical model available, see (Barmish 1994; Bhattacharyya et al. 1995). The popular group of uncertain systems is known as the systems with parametric uncertainty, which means the model structure is fixed but its parameters can vary, typically within some prescribed intervals. Then, the natural task is to find a controller, called a robust controller, that ensures the preserving some important closed-loop properties (e.g. stability) for the whole assumed family of controlled plants, see (Grimble 2006).

The system under the consideration is the Continuous Stirred Tank Reactor (CSTR) with the cooling in the jacket. The mathematical model of this system is described by the set of four nonlinear Ordinary Differential Equations (ODE). This set can be solved by standard numerical methods that are implemented in mathematical software such as Matlab, Simulink etc.

The main aim of this paper is in the design a robustly stabilizing controller for the CSTR with the cooling in the jacket, modelled as a system with parametric uncertainty, by means of algebraic approach. The work will put emphasis on the relatively easily tunable and applicable conventional PID controllers. The robust stabilization and control are verified and discussed by a simulation example of nonlinear CSTR.

CONTINUOUS STIRRED TANK REACTOR

The nonlinear controlled system under the consideration is a CSTR display of which can be found in Figure 1. The so-called Van der Vusse reaction described by general scheme:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$2A \xrightarrow{k_3} D$$
(1)

is performed inside the reactor.

This system can be described by a nonlinear mathematical model derived with the commonly used simplifications that reduce complexity of the system that has a lot of variables and connections. If we introduce these simplifications, the originally very complex system can be described by the set of nonlinear ordinary differential equations – see e.g. (Russell and Denn 1972) or (Vojtesek et al. 2017):

$$\frac{dc_{A}}{dt} = \frac{q_{r}}{V_{r}} (c_{A0} - c_{A}) - k_{1}c_{A} - k_{3}c_{A}^{2}$$

$$\frac{dc_{B}}{dt} = -\frac{q_{r}}{V_{r}}c_{B} + k_{1}c_{A} - k_{2}c_{B}$$

$$\frac{dT_{r}}{dt} = \frac{q_{r}}{V_{r}} (T_{r0} - T_{r}) - \frac{h_{r}}{\rho_{r}c_{pr}} + \frac{A_{r}U}{V_{r}\rho_{r}c_{pr}} (T_{c} - T_{r}) \qquad (2)$$

$$\frac{dT_{c}}{dt} = \frac{1}{m_{c}c_{pc}} (Q_{c} + A_{r}U(T_{r} - T_{c})),$$
where $0 \le c_{A}, 0 \le c_{B}$

This set is derivate with the help of material and heat balances inside the reactor. Variable t in the set of Ordinary Differential Equations (ODE) (2) denotes the time, c are concentrations, T represents temperatures, c_p is used for specific heat capacities, q_r means volumetric flow rate of the reactant, Q_c is heat removal of the cooling liquid, V are volumes, ρ stands for densities, A_r is the heat exchange surface and U is the heat transfer coefficient. Indexes (\bullet)_A and (\bullet)_B belong to compounds A and B, respectively, (\bullet)_r denotes the reactant mixture, (\bullet)_c cooling liquid and (\bullet)₀ are feed (inlet) values.



Figure 1: Continuous stirred tank reactor with cooling in the jacket

This reactor belongs to the class of *lumped-parameter* nonlinear systems, see e.g. Ingham et al. (2000). Nonlinearity can be found in reaction rates (k_j) , which are described via the Arrhenius law:

$$k_{j}(T_{r}) = k_{0j} \cdot \exp\left(\frac{-E_{j}}{RT_{r}}\right), \text{ for } j = 1, 2, 3$$
(3)

where k_0 represent pre-exponential factors and E are activation energies.

The reaction heat (h_r) in Eq. (2) is expressed as:

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B + h_3 \cdot k_3 \cdot c_A^2 \tag{4}$$

where h_i means reaction enthalpies.

The initial conditions for the set of ODE (2) are

$$c_{A}(0) = c_{A}^{s}, c_{B}(0) = c_{B}^{s}, T_{r}(0) = T_{r}^{s}, T_{c}(0) = T_{c}^{s}$$
(5)

The mathematical model of the system described by the set of ODE in Eq. (2) shows that this model has four state variables: $c_A(t)$, $c_B(t)$, $T_r(t)$ and $T_c(t)$. From the control point of view, several input variables can be used, e.g. input concentration of compound A, c_{A0} , input temperature of the reactant, T_{r0} , etc. However, the physical viability of these variables is greatly limited from the practical point of view. That is why are simulation studies mainly focused on the volumetric flow rate of the reactant q_r and the heat removal of the cooling liquid Q_c . The change of both quantities can be practically represented for example by the turn of the valve on the inlet pipe, or by the speed of the pump. Fixed parameters of CSTR are given in Table 1.

Table 1: Parameters of CSTR

Name of the parameter	Symbol and value of the
Volume of the reactor	$V = 0.01 \ m^3$
Density of the reactor	$v_r = 0.01 m$
	$\rho_r = 934.2 \text{ kg.m}^2$
Heat capacity of the	$c_{pr} = 3.01 \text{ kJ.kg}^{-1} \text{.K}^{-1}$
reactant	<u> </u>
Weight of the coolant	$m_c = 5 \ kg$
Heat capacity of the	$c_{pc} = 2.0 \ kJ.kg^{-1}.K^{-1}$
coolant	
Surface of the cooling	$A_r = 0.215 \ m^2$
jacket	
Heat transfer coefficient	$U = 67.2 \ kJ.min^{-1}m^{-2}K^{-1}$
Pre-exponential factor	$k_{01} = 2.145 \cdot 10^{10} min^{-1}$
for reaction 1	
Pre-exponential factor	$k_{02} = 2.145 \cdot 10^{10} min^{-1}$
for reaction 2	
Pre-exponential factor	$k_{03} = 1.5072 \cdot 10^8 \text{ min}^{-1}$
for reaction 3	¹ .kmol ⁻¹
Activation energy of	$E_1/R = 9758.3 K$
reaction 1 to R	
Activation energy of	$E_2/R = 9758.3 K$
reaction 2 to R	2
Activation energy of	$E_3/R = 8560 K$
reaction 3 to R	
Enthalpy of reaction 1	$h_1 = -4200 \ kJ.kmol^{-1}$
Enthalpy of reaction 2	$h_2 = 11000 \ kJ.kmol^{-1}$
Enthalpy of reaction 3	$h_3 = 41850 \ kJ.kmol^{-1}$
Input concentration of	$c_{40} = 5.1 \ kmol.m^{-3}$
compound A	
Input temperature of the	$T_{r0} = 387.05 K$
reactant	

STATIC AND DYNAMIC ANALYSES

Once we have mathematical model of the system, we can make simulation experiments that help with the understanding of the system's behaviour. Also, we can use this knowledge in the design of the controller which will be also described later in the Adaptive control section.

Steady-State Analysis

The steady-state analysis as the first step means that we want to know value of state variables, in our case concentrations c_A , c_B and temperatures T_r , T_c in so called steady-state. The mathematical meaning of this claim is the derivatives with respect to time in the set of ODE (2) are set to zero. It means that the set of ODE (2) is transformed to the set of nonlinear algebraic equations

$$c_{A}^{s} = \frac{-\left(\frac{q_{r}}{V_{r}} + k_{1}\right) \pm \sqrt{\left(\frac{q_{r}}{V_{r}} + k_{1}\right)^{2} - \left(4 \cdot k_{3} \cdot \left(-\frac{q_{r}}{V_{r}}c_{A0}\right)\right)}}{2 \cdot k_{3}};$$

$$c_{B}^{s} = \frac{k_{1} \cdot c_{A}^{s}}{k_{2} + \frac{q_{r}}{V_{r}}};$$

$$T_{r}^{s} = \frac{\frac{q_{r}}{V_{r}}T_{r0} - \frac{h_{r}}{\rho_{r} \cdot c_{pr}} + \frac{U \cdot A_{r}}{\rho_{r} \cdot c_{pr} \cdot V_{r}}T_{c}^{s}}{\frac{q_{r}}{V_{r}} + \frac{U \cdot A_{r}}{\rho_{r} \cdot c_{pr} \cdot V_{r}}};$$

$$T_{c}^{s} = \frac{Q_{c}}{U \cdot A_{r}} + T_{r}$$
(6)

That can be solved numerically for example with the use of simple iteration method. We can observe the steadystate behaviour for various input variables.

Results for various values of volumetric flow rate of the reactant, q_r , and heat removal of coolant, Q_c , are shown in Figure 2.



Figure 2: Steady-state analysis for various volumetric flow rate of the reactant, q_r , and heat removal of the cooling, Q_c

We can read from graphs, that this system has strongly nonlinear behaviour. The optimal working point can be represented by the combination of the volumetric flow rate of the reactant $q_r^s = 2.365 \cdot 10^{-3} m^3.min^{-1}$ and the heat removal $Q_c^s = -18.56 \ kJ.min^{-1}$.

The dynamic analysis and the control is then performed around this working point where steady-state values of state variables are

$$c_A^s = 2.1403 \ kmol.m^{-3}, \ c_B^s = 1.0903 \ kmol.m^{-3}$$

 $T_r^s = 387.34 \ K, \qquad T_c^s = 386.06 \ K$ (7)

Dynamic Analysis

Once we have optimal working point from the steadystate analysis, we can continue with the dynamic analysis which means observing of the system's behaviour after the step change of the input variable. In our case, we have chosen the step changes of the coolant's heat removal, ΔQ_c , because this input will be than used as an action value for the control.

Investigated output variables are output concentration of the product *B*, $c_B(t)$, and output temperature of the coolant, $T_r(t)$. Both values are related to their steadystate values in (7) because we want to display these output from zero and as we can see in (5), these values are initial values in the numerical solution. Input and output variables are then:

$$u(t) = \frac{Q_c(t) - Q_c^s}{Q_c^s} \cdot 100 [\%]$$

$$y_1(t) = c_B(t) - c_B^s [kmol.m^{-3}]$$

$$y_2(t) = T_r(t) - T_r^s [K]$$
(8)

Mathematically, the dynamic analysis means numerical solution of the set of ODE (2) together with (3) and (4). This numerical solution can be easily performed with build-in functions in Matlab or other mathematical software. Results are shown in Figure 3.



Figure 3: Results of the dynamic analysis for various step changes of input variable u(t)

Both courses of output variables $y_1(t)$ and $y_2(t)$ shows nonlinearity of the system which is obvious mainly for the output $y_1(t)$. On the other hand, output $y_1(t)$ can be expressed by the second order transfer function

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{a_2 s^2 + a_1 s + a_0}$$
(9)

This output will be used as a controlled output in the control section of this paper.

ROBUST CONTROL

Models with Parametric Uncertainty

Systems with parametric uncertainty represent an effective and popular way of considering the uncertainty in the mathematical model of a real plant, see e.g. (Barmish 1994) or (Matušů and Prokop 2013; 2014). The utilization of such models supposes known structure (and order) of the transfer function but not precise knowledge of real parameters, which can be bounded by intervals with minimal and maximal possible values. They can be described by a transfer function:

$$G(s,q) = \frac{b(s,q)}{a(s,q)} \tag{10}$$

where b(s,q) and a(s,q) denote polynomials in *s* (Laplace transform) with coefficients depending on *q*, which is a vector of real uncertain parameters. Typically, this vector is confined by some uncertainty bounding set, which is generally a ball in some appropriate norm. The combination of the uncertain system (e.g. transfer function (10)) with an uncertainty bounding set gives the so-called family of systems, see e.g. (Barmish 1994). A special and frequent case of a system with parametric uncertainty is an interval plant. Its parameters vary independently on each other within given bounds, i.e.:

$$G(s,b,a) = \frac{\sum_{i=0}^{m} \left[b_i^-; b_i^+ \right] s^i}{\sum_{i=0}^{n} \left[a_i^-; a_i^+ \right] s^i}$$
(11)

where $b_i^-, b_i^+, a_i^-, a_i^+$ represent lower and upper limits for parameters of numerator and denominator, respectively.

Control Structure and Design

The 2DOF closed-loop control system with separated feedback and feedforward parts of the controller is depicted in Figure 4. The transfer functions G(s), $C_b(s)$, and $C_f(s)$ represent controlled plant, feedback part of the controller, respectively and the signals w(s), n(s), and v(s) are reference, load disturbance, and disturbance signal.



Figure 4: Two-degree-of-freedom control loop

The traditional (one degree of freedom) feedback system is obtained by R=Q. However, there are much relevant evidence that the feedforward part brings positive improvements in control responses, see e.g. (Gorez 2003) or (Matušů and Prokop 2013; 2014).

The control synthesis itself is based on the algebraic ideas of Vidyasagar (1985), and Kučera (1993). Subsequently, the specific tuning rules have been developed and analyzed e.g. in (Prokop and Corriou 1997) or (Matušů and Prokop 2013; 2014).

Besides, the controller tuning rules for the case of law order controlled plant under assumption of either purely reference tracking problem or reference tracking and load disturbance rejection together have been already studied e.g. (Kučera 1993) or (Matušů and Prokop 2013; 2014) and so this part presents the important results and then it is applied to the CSTR as a plant with parametric uncertainty.

First, the control design technique supposes the description of linear systems in Fig. 3 by means of the ring of proper and stable rational functions (R_{PS}). The conversion from the ring of polynomials to R_{PS} can be performed very simply – see e.g. (Vidyasagar 1985) or (Prokop and Corriou 1997) according to:

$$G(s) = \frac{b(s)}{a(s)} = \frac{\frac{b(s)}{(s+m)^n}}{\frac{a(s)}{(s+m)^n}} = \frac{B(s)}{A(s)},$$
(12)

m > 0, $n = \max \{ \deg(a), \deg(b) \}$

The parameter m > 0 will be later used as a controllertuning knob. The value of the tuning knob has a relevant influence on the control behavior of control responses.

The algebraic analysis (Prokop and Corriou 1997; Matušů and Prokop 2013; 2014) leads to the first Diophantine equation:

$$A(s)P(s) + B(s)Q(s) = 1$$
(13)

with a general solution $P(s) = P_0(s) + B(s)T(s)$, $Q(s) = Q_0(s) - A(s)T(s)$, where T(s) is an arbitrary member of (the ring) R_{PS} and the pair $P_0(s)$, $Q_0(s)$ represents any particular solution of (13). Since the feedback part of the controller is responsible not only for stabilization but also for disturbance rejection, the convenient controller from the set of all stabilizing ones can be chosen on the basis of divisibility conditions. The requirement of the reference tracking is obtained by the second Diophantine equation (see Kučera, 1993, Matušů and Prokop, 2013, 2014):

$$F_{w}(s)Z(s) + B(s)R(s) = 1$$
 (14)

Robust Stability

The stability of the feedback loop is a crucial requirement in all control applications. Naturally, the feedback loop can be stable when the controlled and/or control plant is unstable. In the case of uncertainty of controlled plants, robust stability means that not only one fixed closed-loop system is stable but also the whole

family of closed-loop control systems is ensured to be stable. Details can be found in e.g. (Ackermann 1993; Barmish 1994; Bhattacharyya et al. 1995; Matušů and Prokop 2011; 2013; 2014). This paper utilizes the robust stability tests based on a universal tool known as the value set concept in combination with the zero exclusion condition – see e.g. (Barmish 1994) or (Matušů and Prokop 2011).

ADAPTIVE CONTROL

The adaptive approach in this work is based on the recursive identification of the linearized model described by the transfer function (9) during the control. The control scheme is very similar to 2DOF control configuration in Figure 4 but block G is in this case mathematical model of the controlled system, in our case the set of ODE in (2).

The control synthesis employs pole-placement method together with the spectral factorization. Our previous experiments (for example (Vojtěšek and Dostál 2005; 2016)) have shown, that this method produces sufficient control results.

This control synthesis is based on the solution of the set of Diophantine equations

$$a(s)f(s), \quad)q(s) = d(s)$$

$$t(s)f_w(s) + b(s)r(s) = d(s)$$

(15)

where polynomials a(s) and b(s) are polynomials from the transfer function (9) and they are estimated recursively with the Ordinary recursive least-squares method (Bobál et al. 2005). Polynomial t(s) is auxiliary polynomial and unknown controller's polynomials p(s), q(s) and r(s) are computed from (16).

Unknown stable polynomial d(s) on the right side of equations (16) was designed with the use of poleplacement method, e.g. this polynomial is generally

$$d(s) = \prod_{i=1}^{\deg d(s)} (s+s_i)$$
(16)

where $s_i = \alpha_i + \omega_i j$ are roots of the polynomial and choice of these roots affects control results. More details about this method can be found for example in (Vojtěšek and Dostál 2005).

SIMULATIONS AND DISCUSSION

A Robust Approach

The CSTR was identified in (Vojtěšek et al. 2017) as a second order system with the transfer function (9) with nominal parameters: $a_2 = 1$, $a_1 = 1.4550$, $a_0 = 0.3072$, $b_1 = -0.0037$, $b_0 = -0.0095$. The intervals for uncertain perturbations were obtained by deeper analysis of the dynamic behavior and they result in the following ones:

$$a_{0} = [0.24576; 0.36864],$$

$$a_{2} = [0.8; 1.2], a_{1} = [1.164; 1.746],$$

$$b_{1} = [-0.00296; -0.00444], b_{0} = [-0.0076; -0.0114]$$
(17)

Three 2DOF controllers have been designed for the nominal plant and the tuning parameters. The first one was generated for m = 0.5, the second one for m = 0.8 and the third one for m = 1.2. The feedback and feedforward parts of the controller for the first one is:

$$C_{b}(s) = \frac{q_{2}s^{2} + q_{1}s + q_{0}}{s^{2} + p_{1}s} = \frac{-61.3653s^{2} - 39.7878s - 6.5789}{s^{2} + 0.3179s}$$
(18)
$$C_{f}(s) = \frac{r_{2}s^{2} + r_{1}s + r_{0}}{s^{2} + p_{1}s} = \frac{-26.3158s^{2} - 26.3158s - 6.5789}{s^{2} + 0.3179s}$$

Figure 5 and Figure 6 show the controlled and control variables for all three tuning parameters. The red lines depict the nominal plant responses and black shadows are responses for the whole uncertain family (17), represented by $3^5=243$ members (three values for each interval parameter: minimum, midpoint, and maximum). The load disturbance n = 10 was injected in the time t = 150 and it is evident that no permanent error is observed.



Figure 5: Set of output controlled variables for *m*=0.5 (left), *m*=0.8 (middle), and *m*=1.2 (right)



Figure 6: Set of input control variables for *m*=0.5 (left), *m*=0.8 (middle), and *m*=1.2 (right)

Simulation results proved that the fix robust controller could be designed for a wide family of interval systems. The results are shown in Figures 5 and 6 for three values of the tuning parameter m>0. The choice of the tuning parameter m > 0was found empirically and experimentally. Until now, there is no exact theory on how to obtain the optimal value (see e.g. Prokop and Corriou, 1997). The Figure 7 shows the zoomed value sets for all three values of m. All three subfigures from Figure 7 may seem the same for the first sight, but please note the differences in axes ranges. Anyway, they confirm the robust stability of the designed control loops since they are excluded from the critical point (0,0j) and all required preconditions are fulfilled (Barmish 1994).



Figure 7: Zoomed value sets for *m*=0.5 (left), *m*=0.8 (middle) and *m*=1.2 (right)

In order to verify the practical usability of the designed controllers, they were applied not only to the linearized model, but also to the original nonlinear model of CSTR. The control results for this nonlinear case are shown and mutually compared in Figure 8.



Figure 8: Robust control of the original nonlinear model for three values of m – comparison of the output controlled variables (left) and the input control variables (right)

The control results shown in Figure 8 assumes that there is no limitation of the control signal. On the other hand, Figure 9 provides the control behavior for the same controllers, but with the saturated control signals in the range ± 100 %. It can be seen that this saturation affects the signals for m=0.8 and m=1.2. Consequently, higher peaks caused by the wind-up effect are observable, especially for m=1.2.





An Adaptive Approach

Three adaptive controllers for 2DOF configuration were tuned, assuming the placement of the closed-loop poles 0.07, 0.1, and 0.2, respectively. Figure 10 shows the control results for the original nonlinear CSTR model, and Figure 11 presents the evolution of the identified parameters during the simulation.



Figure 10: Adaptive control results – output (left) and control (right) signals



Figure 11: Adaptive control results – identified parameters

Comparison and Discussion

The control performance of both robust and adaptive approaches can be tuned by the parameter m or the proper pole-placement. In all cases, the costs for the rapid control and better disturbance rejection are the higher and more aggressive control signals. For some faster robust controllers, the control signals would have to be restricted for the practical application. The main advantage of the self-tuning controllers is obvious from its name, i.e., after successful initialization, they are able to control the CSTR without knowledge of the model. On the other hand, the main advantage of the off-line tuned robust controllers is their simplicity and reliability, even under prescribed model uncertainty. The comparison of control results for two reasonable choices of tuning parameters, i.e., m=0.5 for the robust controller, and $\alpha=0.2$ for the adaptive controller, are shown in Figure 12. Anyway, it was shown that both approaches are able to control the CSTR satisfactorily and the final choice of the approach depends on the additional requirements or preferences of a user or control engineer.



Figure 12: Comparison of selected robust and adaptive controllers – output (left) and control (right) signals

CONCLUSIONS

Modelling and control of CSTR are addressed in the contribution. Two different approaches of control were designed and compared. The first one is an adaptive self-tuning principle based on the recursive identification procedure with polynomial control design. The second control principle utilizes robust control algorithms designed in the ring R_{PS}. The synthesis method itself is based on linearized model with parametric uncertainty and accompanied by the analysis of robust stability. Both approaches use the 2DOF feedback control structure. As an application, a set of designed robust and adaptive controllers were applied to

control of an original nonlinear model of CSTR. The main aim of the control design was energy saving in the industry operation of CSTR. All simulations were performed in the MATLAB and Simulink environment.

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