CHEMICAL ENGINEERING TRANSACTIONS
VOL. 81, 2020

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Qiuwang Wang, Min Zeng, Panos Seferlis, Ting Ma, Jiří J. Klemeš

ISBN 978-88-95608-79-2; **ISSN** 2283-9216

DOI: 10.3303/CET2081135

Feedback Control of Chemical Reactors by Modern Principles

Roman Prokop[a,*], Radek Matušů[b], Jiří Vojtěšek[c]

[a]Department of Mathematics, Faculty of Applied Informatics, Tomas Bata University in Zlín, Nad Stráněmi 4511, 76005 Zlín, Czech Republic
[b]Centre for Security, Information and Advanced Technologies (CEBIA-Tech), Faculty of Applied Informatics, Tomas Bata University in Zlín, Nad Stráněmi 4511, 76005 Zlín, Czech Republic
[c]Department of Process Control, Faculty of Applied Informatics, Tomas Bata University in Zlín, Nad Stráněmi 4511, 76005 Zlín, Czech Republic
prokop@utb.cz

Plug-Flow Reactors (PFR) belong to frequently used technological plants which exhibit unpleasant behavior. The traditional PID control structure in these cases may fail or demonstrate an unacceptable behavior. The paper brings another approach of control design called robust. It means that the controller is fixed but resistant to the uncertainty of the controlled plant. The studied approach considers a linear system with parametric uncertainty, which covers a family of all feasible plants. A controller with fix parameters is then designed so that for all possible plants, the acceptable stable control behavior is obtained. The structure of the control law is in two degree of freedom (2DOF) which offers better control responses than classical structures. All calculations and simulations of mathematical models and control responses were performed in the Matlab and Simulink environment.

1. Introduction

Various kinds of chemical reactors play a fundamental role in the chemical and biochemical industry. Usually they have nonlinear behavior that causes difficulties in the control of processes inside the reactors. Other unpleasant property can be found in the complexity of such processes with heat and kinetic mechanism, lot of variables and properties that result in a non-linear mathematical description. This unpleasant property can be overcome with the linearization and simplifications that reduce the intricacy of the system. On the other hand, this simplification can result in an inaccurate description of the system. As a consequence, the conventional linear control with fixed parameters can be questionable or unacceptable. The solution should be found in so-called advanced control approaches like Adaptive, Robust, Fuzzy or Artificial Intelligent methods.
The utilization of adaptive (e.g., self-tuning) schemes brings more difficult, clumsy and time-consuming computations (Åström and Wittenmark, 2008). The control design using a hybrid adaptive control principle was used in Vojtesek et al. (2017) where the originally non-linear system was represented by the 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. There are more ways of incorporating the uncertainty into the mathematical model available as in Bhattacharyya (2017). 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. 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 as in Barmish (1994).
The main aim of this paper is in the design a robustly stabilizing controller for the PFR with the cooling in the jacket, modelled as a system with parametric uncertainty, using the algebraic approach. In Section 2, a mathematical model of PFR is described. Section 3 outlines principles of uncertainty, robust control and control design in the ring of proper and stable rational functions (R_{PS}). Section 4 is devoted to simulation example and discussion of results. Section 5 offers some concluding remarks.

Paper Received: 22/04/2020; Revised: 04/06/2020; Accepted: 11/06/2020
Please cite this article as: Prokop R., Matušů R., Vojtěšek J., 2020, Feedback Control of Chemical Reactors by Modern Principles, Chemical Engineering Transactions, 81, 805-810 DOI:10.3303/CET2081135

2. Plug-flow reactor

The studied simulation model is a tubular chemical reactor with the ideal plug-flow chemical reaction with a simple exothermic consecutive reaction *A → B → C* in the liquid phase and with cooling in the jacket. These types of reactors are called PFRs. The mathematical description of all quantities and relations among them is quite complex, and some simplifications are necessary. Heat losses and conduction along the metal wall of the pipes are neglected, and the heat transfer through the wall is consequential for the dynamic study. All densities, heat capacities and heat transfer coefficients are expected to be constant. Two types of cooling can be used in the jacket – *co-current* (solid black line) and *counter-current cooling* (red dashed line). The differences between them are displayed in Figure 1, and they will be investigated in static and dynamic analyses.

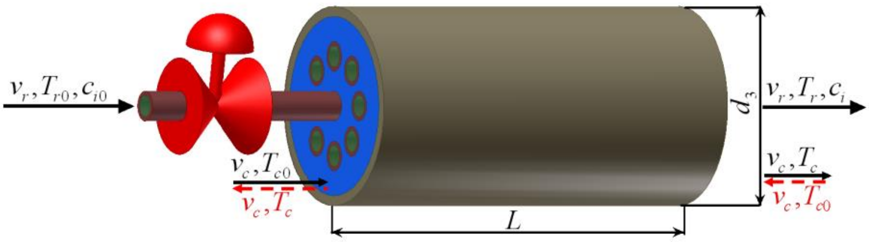

Figure 1: PFR with co-current and counter-current cooling in the jacket – the main pipe

The jacket has diameter d_3, and the outer diameter of each pipe is d_2, while the inner diameter is denoted as d_1 – see Figure 2.

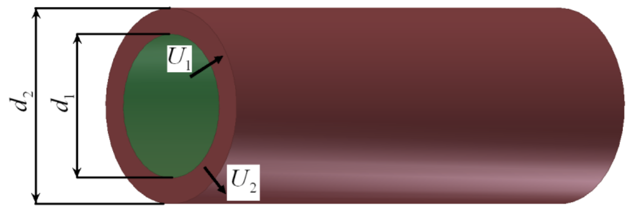

Figure 2: PFR – one pipe

The mathematical description of the system is based on material and heat balances inside the reactor. The mathematical model is then described by a set of Partial Differential Equations (PDE):

$$\begin{aligned}
&\frac{\partial c_A}{\partial t} + v_r \cdot \frac{\partial c_A}{\partial z} = -k_1 \cdot c_A \\
&\frac{\partial c_B}{\partial t} + v_r \cdot \frac{\partial c_B}{\partial z} = k_1 \cdot c_A - k_2 \cdot c_B \\
&\frac{\partial T_r}{\partial t} + v_r \cdot \frac{\partial T_r}{\partial z} = \frac{h_r}{\rho_r \cdot c_{pr}} - \frac{4 \cdot U_1}{d_1 \cdot \rho_r \cdot c_{pr}} \cdot (T_r - T_w) \\
&\frac{\partial T_w}{\partial t} = \frac{4}{\left(d_2^2 - d_1^2\right) \cdot \rho_w \cdot c_{pw}} \cdot \left[d_1 \cdot U_1 \cdot (T_r - T_w) + d_2 \cdot U_2 \cdot (T_c - T_w) \right]
\end{aligned} \tag{1}$$

The last PDE for co-current cooling and counter-current cooling (opposite flow of the cooling medium) are denoted as

$$\begin{aligned}
&\frac{\partial T_c}{\partial t} + v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2}{\left(d_3^2 - n_1 \cdot d_2^2\right) \cdot \rho_c \cdot c_{pc}} (T_w - T_c) \\
&\frac{\partial T_c}{\partial t} - v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2}{\left(d_3^2 - n_1 \cdot d_2^2\right) \cdot \rho_c \cdot c_{pc}} (T_w - T_c)
\end{aligned} \tag{2}$$

where T is the temperature, d represents diameters, ρ are densities, c_p means specific heat capacities, U stands for the heat transfer coefficients, n_1 is a number of tubes and L represents the length of the reactor. Index $(\bullet)_r$ means the reaction compound, $(\bullet)_w$ is for the metal wall of the pipes and $(\bullet)_c$ for the cooling liquid. Variables v_r and v_c are fluid velocities of the reactant and cooling liquid as:

$$v_r = \frac{q_r}{f_r}; \quad v_c = \frac{q_c}{f_c}, \; where \quad f_r = n_1 \cdot \frac{\pi \cdot d_1^2}{4}; \quad f_c = \frac{\pi}{4}\left(d_3^2 - n_1 \cdot d_2^2\right) \tag{3}$$

where q is flow rates and f are constants. The reaction velocities, k_i, in Eqs(1), (3) are non-linear functions of temperature computed via the Arrhenius law:

$$k_j = k_{oj} \cdot \exp\left(-\frac{E_j}{R \cdot T_r}\right), \text{for } j = 1,2 \tag{4}$$

where k_{0j} represents pre-exponential factors, E means activation energies and R is the gas constant. h_r in the third equation is the reaction heat computed as

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B \tag{5}$$

where h_j is used for reaction enthalpies.

The mathematical model given by Eq(1) to Eq(5) shows that this plant is a *nonlinear system with continuously distributed parameters*. Strong nonlinearity can be found in Eq(4), and the system is with distributed parameters because of the presence of the PDE where the state variable is related not only to the time variable, t, but the space varibable, z, too. The initial conditions are $c_A(z,0) = c_A^s(z)$, $c_B(z,0) = c_B^s(z)$, $T_r(z,0) = T_r^s(z)$, $T_w(z,0) = T_w^s(z)$ and $T_c(z,0) = T_c^s(z)$ and boundary conditions $c_A(0,t) = c_{A0}(t)$,$c_B(0,t) = c_{B0}(t) = 0$, $T_r(0,t) = T_{r0}(t)$, $T_c(0,t) = T_{c0}(t)$ for the co-current cooling and $T_c(0,t) = T_{c0}(t)$ for the counter-current cooling. Fixed parameters of PFR (see Dostál et al., 1996) are displayed in Table 1.

Table 1: Parameters of PFR

Name of the parameter	Symbol and value of the parameter
Inner diameter of the pipe	$d_1 = 0.02$ *m*
Outer diameter of the pipe	$d_2 = 0.024$ *m*
Diameter of the jacket	$d_3 = 1$ *m*
Number of pipes	$n_1 = 1200$
Length of the reactor	$L = 6$ *m*
Density of the reactant	$\rho_r = 985$ $kg.m^3$
Density of the pipe's wall	$\rho_w = 7{,}800$ $kg.m^3$
Density of the cooling liquid	$\rho_c = 998$ $kg.m^3$
Heat capacity of the reactant	$c_{pr} = 4.05$ $kJ.kg^{-1}.K^{-1}$
Heat capacity of the pipe's wall	$c_{pw} = 0.71$ $kJ.kg^{-1}.K^{-1}$
Heat capacity of the cooling liquid	$c_{pc} = 4.18$ $kJ.kg^{-1}.K^{-1}$
Heat transfer coefficient: reactant-wall	$U_1 = 2.8$ $kJ.m^{-2}.K^{-1}.s^{-1}$
Heat transfer coefficient: wall-cooling liquid	$U_2 = 2.56$ $kJ.m^{-2}.K^{-1}.s^{-1}$
Pre-exponential factor for reaction 1	$k_{10} = 5.61 \times 10^{16}$ s^{-1}
Pre-exponential factor for reaction 2	$k_{20} = 1.128 \times 10^{16}$ s^{-1}
Activation energy of reaction 1 to R	$E_1/R = 13{,}477$ *K*
Activation energy of reaction 2 to R	$E_2/R = 15{,}290$ *K*
Enthalpy of reaction 1	$h_1 = 5.8 \times 10^4$ $kJ.kmol^{-1}$
Enthalpy of reaction 2	$h_2 = 1.8 \times 10^4$ $kJ.kmol^{-1}$
Input concentration of compound A	$c_{A0}^s = 2.85$ $kmol.m^{-3}$
Input temperature of the reactant	$T_{r0}^s = 323$ *K*
Input temperature of the cooling liquid	$T_{c0}^s = 293$ *K*

This system has five state variables – concentrations $c_A(z,t)$, $c_B(z,t)$ and temperatures $T_r(z,t)$, $T_w(z,t)$ and $T_c(z,t)$. Input and output variables are defined as

$$u(t) = \frac{q_c(t) - q_c^s}{q_c^s} \cdot 100, \quad [\%], \qquad y(t) = T_{mean}(t) = \frac{\sum_{z=1}^{N} T_r(z,t)}{N}, \quad [K] \tag{6}$$

Where the output variable is the mean variable of reactive temperature T_r.

3. Robust control

Parametric uncertainty of models is outlined in Section 3.1, while the control synthesis is described in Section 3.2. Section 3.3 deals with the basic facts about robust stability.

3.1 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, as considered in Matušů and Prokop (2013). 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 ratio of two polynomials (transfer function) *G(s,q) = b(s,q)/a(s,q)*, 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 with an uncertainty bounding set gives the so-called family of systems as in Barmish (1994). A uniquel and frequent case of a system with parametric uncertainty is interval plants. Its parameters can vary independently on each other within given bounds, i.e.: $a_i \in [a_i^-; a_i^+], b_i \in [b_i^-; b_i^+]$, where $b_i^-, b_i^+, a_i^-, a_i^+$ represent lower and upper limits for parameters of numerator and denominator.

3.2 Control structure and design

For the control design, the 2DOF closed-loop system with separated feedback and feedforward parts of the controller was chosen, see Kučera (1993), and the control law is governed by:

$$P(s)U(s) = R(s)W(s) - Q(s)Y(s) \tag{7}$$

The transfer functions *G(s) =B(s)/A(s),* $C_b(s)=Q(s)/P(s)$, and $C_f(s)=R(s)/Q(s)$ represent the controlled plant, feedback part of the controller, and feedforward part of the controller and the signals *w*(*s*), *n*(*s*), and *v*(*s*) are reference, load disturbance, and disturbance signal. The traditional (one degree of freedom) feedback system is obtained by *R*=*Q.* However, there are many relevant evidence that the feedforward part brings positive improvements in control responses, as considered in the work of Gorez, (2003). The control synthesis itself is based on the algebraic ideas of Kučera (1993). The specific tuning rules have been developed and analyzed by Prokop and Corriou (1997). The controller tuning rules for the case of law order controlled plant under the assumption of either pure reference tracking problem or reference tracking and load disturbance rejection together have been already studied by Matušů and Prokop (2013). The control design technique supposes the description of linear systems using R_{PS}. The conversion from the ring of polynomials to R_{PS} can be performed very simply (see e.g. Prokop and Corriou, 1997) according to:

$$G(s) = \frac{b(s)}{a(s)} = \frac{b(s)/(s+m)^n}{a(s)/(s+m)^n} = \frac{B(s)}{A(s)}, \quad m > 0,\ n = \max\{\deg(a), \deg(b)\} \tag{8}$$

The parameter $m > 0$ will be later used as a controller-tuning knob. The value of the tuning knob has important influence on the control behavior of control responses. The algebraic analysis, see e.g. Prokop and Corriou, (1997) or Matušů and Prokop (2014) leads to the first Diophantine equation:

$$A(s)P(s) + B(s)Q(s) = 1 \tag{9}$$

with a general solution $P(s)=P_o(s)+B(s)T(s)$, $Q(s)=Q_o(s)-A(s)T(s)$, where *T*(*s*) is an arbitrary member of R_{PS} and the pair $P_o(s)$, $Q_o(s)$ represents any particular solution of Eq(9). This principle is known as Youla – Kučera parameterization of all stabilizing controllers. All possible solutions of the Diophantine equation give all stabilizing feedback controllers. 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 based on divisibility conditions. The requirement of the reference tracking is obtained by the second Diophantine equation (F_w is the reference denominator) (Kučera 1993):

$$F_w(s)Z(s) + B(s)R(s) = 1 \tag{10}$$

3.3 Robust stability

Stability of the feedback loop is the crucial requirement in all control applications. Naturally, the feedback loop can be stabilized even if the controlled and/or control systems are 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. Since the stability of linear systems can be investigated using the stability of its characteristic polynomials, the main object of interest from the robust stability

viewpoint is the uncertain continuous-time closed-loop characteristic polynomial $p(s,q)=\Sigma\, \rho_i(q)\, s^i$. Details can be found in the work of Bhattacharyya (2017).
However, there is a universal graphical approach applicable for all, even in complicated cases. It is known as the value set concept in combination with the zero exclusion condition as considered in the work of Matušů and Prokop (2011). In other words, $p(j\omega,Q)$ is the image of Q under $p(j\omega, .)$. Practical construction of the value sets then means to substitute s for $j\omega$, fix ω and let the vector of uncertain parameters q range over the set Q. The zero exclusion condition for Hurwitz stability of a family of continuous-time polynomials says (Barmish, 1994): Assume invariant degree of polynomials in the family, pathwise connected uncertainty bounding set Q, continuous coefficient functions ρ_i(q) for $i = 0,1,2,K,n$ and at least one stable member $p(s,q^o)$. The family P is robustly stable if and only if the complex plane origin is excluded from the value set $p(j\omega,Q)$ at all frequencies $\omega \geq 0$, that is P is robustly stable if and only if $0 \notin p(j\omega,Q),\ \forall\omega \geq 0$.

4. Simulations and discussion

4.1 Simulation example and results

The PFR controlled object was identified as a second-order system with nominal parameters:

$$G(s)=\frac{b(s)}{a(s)}=\frac{b_1 s+b_0}{s^2+a_1 s+a_0}=\frac{-3.3326\cdot 10^{-4}s-3.1421\cdot 10^{-5}}{s^2+1.4192\cdot 10^{-2}s+5.0208\cdot 10^{-5}} \tag{11}$$

The intervals for uncertain perturbations are obtained by a deeper analysis of the dynamic behavior, and they result in ± 10 % from the nominal ones.
The first 2DOF controller has been designed for the nominal plant and the tuning parameter m = 0.005. The feedback and feedforward parts of the controller are:

$$\begin{aligned} C_b(s)&=\frac{q_2 s^2+q_1 s+q_0}{s^2+p_1 s}=\frac{0.5666s^2-0.0067s-1.9891.10^{-5}}{s^2+0.0056s}, \\ C_f(s)&=\frac{r_2 s^2+r_1 s+r_0}{s^2+p_1 s}=\frac{0.7956s^2-0.0080s-1.9891}{s^2+0.0056s} \end{aligned} \tag{12}$$

The second 2DOF controller is generated by using tuning parameter m = 0.02 in the form:

$$\begin{aligned} C_b(s)&=\frac{q_2 s^2+q_1 s+q_0}{s^2+p_1 s}=\frac{42.0370s^2-0.8816s-0.0051}{s^2+0.0518s}, \\ C_f(s)&=\frac{r_2 s^2+r_1 s+r_0}{s^2+p_1 s}=\frac{12.7303s^2-0.5092s-0.0051}{s^2+0.0518s} \end{aligned} \tag{13}$$

Figure 3 shows the output controlled variables for both tuning parameters. The red lines depict the nominal plant responses, and black shadows are responses for the whole uncertain family (± 10 %). The load disturbance n = 1 was injected in the time t = 6,000 seconds, and it is evident that no permanent error is observed.

4.2 Analysis and discussion

Many simulations were performed in the Simulink environment, and Figure 3 represents only two of them. Simulation results proved that the fix robust controller could be designed for a wide family of interval systems. The choice of the tuning parameter $m > 0$ was found empirically and experimentally. Until now, there is no logical way how to obtain the optimal value (Prokop and Corriou, 1997). To verify the practical usability of both designed controllers, they were applied not only to the linearized model, but also to the original nonlinear model of PFR. The control results for this non-linear case are shown and mutually compared in Figure 3. The left side corresponds to the value m = 0.005, while the right side represents the value m = 0.02. All simulations confirm that lower values of the parameter m give slower responses of the control behaviour. The price for the faster response is the more aggressive (higher) control inputs. It demonstrates the robust stability of both designed control systems.

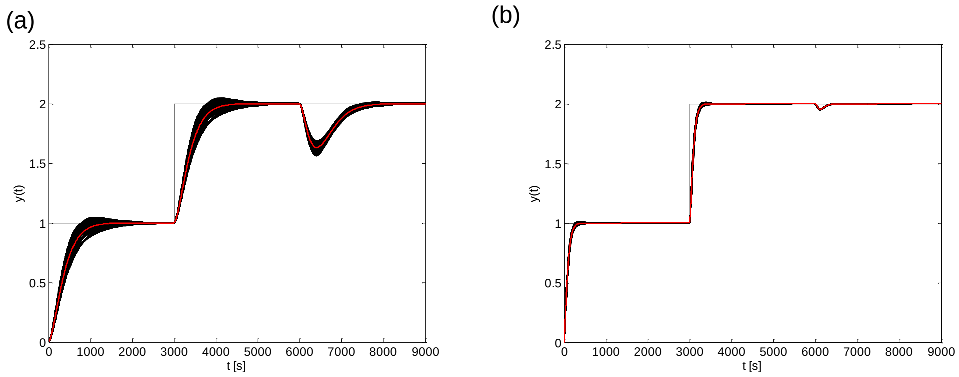

Figure 3: Set of output controlled variables for (a) m=0.005 and (b) m=0.02

5. Conclusions

The paper deals with some applications of continuous-time 2DOF robust control algorithms designed in R_{PS} to systems with parametric uncertainty. The approach brings two novel features. The first one consists in the synthesis method, which utilizes the graphical approach to robust stability analysis based on the value set concept and the zero exclusion condition. The second feature is in the application of the 2DOF structure of the feedback loop. Two designed robust controllers were applied to control of uncertain systems obtained from a non-linear PFR. The future work will be focused on the control of non-linear plants and analysis.

Acknowledgements

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic within the National Sustainability Program; Project No. LO1303 (MSMT-7778/2014) and by the European Regional Development Fund under the project CEBIA-Tech No. CZ.1.05/2.1.00/03.0089.

References

Åström K. J., Wittenmark B., 2008, Adaptive control, 2nd ed., Dover, Mineola, NY, USA.

Barmish B. R., 1994, New tools for robustness of linear systems, Macmillan, New York, USA.

Bhattacharyya S. P., 2017, Robust control under parametric uncertainty: An overview and recent results. Annual Reviews in Control, 44, 45-77.

Dostál P., Prokop R., Prokopová Z., Fikar M., 1996, Control design analysis of tubular chemical reactors. Chemical Papers, 50, 195-198

Gorez R., 2003, New design relations for 2-DOF PID-like control systems. Automatica, 39, 901-908.

Ingham J., Dunn I. J., Heinzle E., Prenosil J. E., 2000, Chemical engineering dynamics. An Introduction to Modeling and Computer Simulation. Second. Completely Revised Edition. VCH Verlagsgesellshaft. Weinheim, Germany. ISBN: 3-527-29776-6

Kučera V., 1993, Diophantine Equations in Control – A survey. Automatica, 29, 1361-1375.

Matušů R., Prokop R., 2011, Graphical analysis of robust stability for systems with parametric uncertainty: an overview. Transactions of the Institute of Measurement and Control, 33, 274-290.

Matušů R., Prokop R., 2013, Algebraic design of controllers for two-degree-of-freedom control structure. International Journal of Mathematical Models and Methods in Applied Sciences, 7, 630-637.

Oravec J., Trafczynski M., Bakosova M., Markowski M., Meszaros A., Urbaniec K., 2017, Robust Model Predictive Control of Heat Exchanger Network in the Presence of Fouling. Chemical Engineering Transactions, 61, 337-342.

Prokop R., Matušů R., Vojtěšek J., 2019, Robust control of continuous stirred tank reactor with jacket cooling. Chemical Engineering Transactions, 76, 787-792.

Prokop R., Corriou J. P., 1997, Design and analysis of simple robust controllers. International Journal of Control, 66(6), 905-921.

Vojtěšek J., Prokop R., Dostál P., 2017, Two degrees-of-freedom hybrid adaptive approach with pole-placement method used for control of isothermal chemical reactor. Chemical Engineering Transactions, 61, 1855-1860.