Tomas Bata University in Zlín

Faculty of Applied Informatics

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Doctoral Thesis

Chemical Reactors: Modern Control Methods

Study-branch: Technical Cybernetics

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Zlín, Czech Republic, 2007

Published by Tomas Bata University in Zlín in 2008.

Key words: CSTR, tubular chemical reactor, modelling, simulation, steady-state analysis, dynamic analysis, adaptive control, predictive control, polynomial methods

Klíčová slova: Průtočný reaktor, trukový reaktor, modelování, simulace, statická analýza, dynamická analýza, adaptivní řízení, prediktivní řízení, polynomiální metody

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The electronic version of the Doctoral Thesis Summary may be found at www.utb.cz.

ISBN 80-……

Acknowledgements

I would like to thank my supervisor, ***Prof. Petr Dostál***, for his support and trust in my abilities. I could not achieve anything without his help.

At the same time I wish to express my sincere gratitude to all my colleagues, especially ***František Gazdoš*** and ***David Sámek***, for giving me professional comments and recommendations concerning my work. My special thanks belong to ***Anežka Lengálová*** who revises English in this work.

And last but not least I would like to thank to my mother, entire family and friends for their support, encouragement and comprehension during my work.

Dedicated to my wife Magdaléna and daughter Julie…

…for their love, support and motivation

RESUMÉ

Cílem disertační práce je návrh a ověření vhodné metody řízení některých typů chemických reaktorů. Chemické reaktory se obecně vyznačují nelineárními vlastnostmi, které jsou ve většině případů značně výrazné. Proto použití konvenčních metod jejich řízení PI resp. PID regulátory s pevně nastavenými parametry může být velmi nekvalitní nebo i nemožné.

Nutným předpokladem úspěšného návrhu řízení procesů této třídy je představa o jejich statických a dynamických vlastnostech. Jednou z možností, jak znalosti o těchto vlastnostech získat je měření na reálném zařízení. Toto ovšem většinou není možné uskutečnit. Jako jediná schůdná cesta se pak jeví statická a dynamická analýza řízeného procesu pomocí simulací, tj. experimentů na jeho matematickém modelu. Simulační metody mají i další výhody oproti experimentům na reálném zařízení, jako jsou menší časové nároky, nižší náklady a hlavně bezpečnost.

Statická analýza procesu ukazuje chování systému v ustáleném stavu což obvykle slouží jako výchozí bod pro volbu optimálního pracovního bodu, tzn. takové kombinace vstupních veličin, při které je produkce maximální s minimálními náklady. Dynamická analýza je dalším krokem po statické analýze a ukazuje chování systému po změně vstupních veličin. Toto chování nám posléze poslouží pro volbu vhodné řídící metody.

V práci jsou použity dvě metody ze třídy tzv. moderních metod řízení.

V prvním případě metoda spojitého adaptivního řízení, založená na volbě externího lineárního modelu (ELM) původně nelineárního systému a použití regulátoru s parametry přestavovanými v závislosti na průběžně identifikovaných parametrech ELM řízeného procesu. Při identifikaci je použita obecně známá metoda nejmenších čtverců spolu s jejími modifikacemi. Při syntéze je v tomto případě použita polynomiální metoda společně s metodou přiřazení pólů a technikou LQ (lineárního kvadatického) řízení. Řízení je uvažováno v konfiguraci s jedním (1DOF) i se dvěma (2DOF) stupni volnosti.

Ve druhém případě je použita metoda založená na zobecněném prediktivním řízení, kde se posloupnost řídících signálů vypočítá na základě minimalizace odchylky výstupní veličiny a žádané veličiny v definovaném budoucím horizontu.

Všechny metody jsou nejdříve ověřeny simulačně na matematických modelech průtočného reaktoru (CSTR) a trubkového reaktoru, ale také praktickým měřením na reálném modelu průtočného chemického reaktoru. Dosažené výsledky ukazují použitelnost navržených metod v reálných systémech.

Klíčová slova: Průtočný reaktor, trukový reaktor, modelování, simulace, statická analýza, dynamická analýza, adaptivní řízení, prediktivní řízení, polynomiální metody

ABSTRACT

Design and verification of suitable methods for control of two types of chemical reactors are the main aims of this work. Chemical reactors are often characterized by highly nonlinear behaviour. In such a case the use of the conventional control strategies that employ PI or PID controllers with fixed parameters can result in poor performance.

Knowledge about the static and dynamic properties is a necessary condition for design of a controller. One possibility how to obtain such information about the system is the investigation of the real system. Unfortunately, measurements on the real system are not always feasible. The only way how to obtain static and dynamic behaviour of these systems is the use of simulation, i.e. experiments on their mathematical model. Simulations have several advantages over experiments on the real system. Among them are the lower costs, increased safety and less time consumption.

Steady-state analysis is usually the first step in the investigation of the system. Steady-state analysis shows the behaviour of the system in the steady state which can help with the choice of the optimal working point, i.e. the appropriate combination of the input variables which results in maximal production with minimal cost. The next step after the steady-state analysis is the dynamic analysis which investigates the dynamic properties of the system. Based on dynamic analysis, the suitable control strategy can be chosen.

Two modern control approaches are investigated in this work. The first approach is the adaptive control which is based on external linear model (ELM) of the originally nonlinear system. The parameters of the model are identified recursively and controller parameters are recomputed in each step. Model parameters are obtained via well-known recursive least-squares method and its modifications. Polynomial, pole-placement and Linear-Quadratic (LQ) approaches are employed for controller synthesis. Two control system configurations are considered during the controller design: one degree-of-freedom (1DOF) and two degrees-of-freedom (2DOF).

The second approach used in this work is the Generalized Predictive Control (GPC) where the future control sequence is computed by the minimizing the error between reference and output signal on the prediction horizon.

All methods were first examined by simulations on mathematical models of two types of chemical reactors – the Continuous Stirred Tank Reactor (CSTR) and the tubular chemical reactor and then verified by measurements on the laboratory model of the CSTR. Results have proved the applicability of the proposed methods on real systems.

Keywords: CSTR, tubular chemical reactor, modelling, simulation, steady-state analysis, dynamic analysis, adaptive control, predictive control, polynomial methods

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LIST OF SYMBOLS AND ABBREVIATIONS

List of Abbreviations

CSTR	Continuous Stirred Tank Reactor
ELM	External Linear Model
CT	Continuous-Time
1DOF	One degree-of-freedom
2DOF	Two degrees-of-freedom
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
ARX	Auto-Regressive eXogenous model
ARMAX	Auto-Regressive Moving Average eXogenous model
FIR	Finite Impulse Response
OE	Output Error
RLS	Recursive Least Squares
BIBO	Bounded Input-Bounded Output
LQ	Linear Quadratic approach
GPC	Generalized Predictive Control
MPC	Model Predictive Control
SISO	Single-Input Single-Output
CARMA	Controller Auto-Regressive Moving-Average model
CARIMA	Controller Auto-Regressive Integrated Moving-Average model
LQ	Linear-Quadratic

PFR	Plug Flow Reactor
PID	Proportional-Integral-Derivative (controller)
USB	Universal Serial Bus
PCT40	Process Control Teaching system
SOL	SOLenoid
PSV	Proportional Solenoid Valve
PC	Personal Computer
I/O	Input/Output
PCI	Peripheral Component Interconnect
NaCl	sodium chloride
$KHCO_3$	potassium bicarbonate

List of symbols

I. THEORETICAL PART

t	time
x	state variable
z	space variable
L	length
$(\cdot)^s$	indicates steady-state
$(\cdot)^0$	indicates initial state
$\alpha_{1,2}$	constants
$\beta_{1,2}$	constants

$\boldsymbol{x}(t)$	state vector
$\boldsymbol{u}(t)$	input vector
$\boldsymbol{f}$	nonlinear vector function
$\boldsymbol{x}^s$	vector of input states
$\boldsymbol{\varphi}$	nonlinear vector function
k	step in iteration
ε_{ss}	accuracy of iteration process
y	output variable
h_i	integration step
$g_{1\text{-}4}$	coefficients in Runge-Kutta's method
h_z	discretization step
i, j	indexes
s	continuous-time complex variable
$a(s)$, $b(s)$	continuous-time polynomials in the transfer function of the system $G(s)$
$u(t)$	continuous input variable
$y(t)$	continuous output variable
σ	differentiation operator
$U(s)$	Laplace transform of the input
$Y(s)$	Laplace transform of the output
$o_1(s)$	polynomial which includes initial conditions
$G(s)$	continuous-time transfer function of the system
$u_f(t)$	filtered input variable
$y_f(t)$	filtered output variable

$c(\sigma)$	filtration polynomial
$o_2(s)$, $o_3(s)$	polynomial of initial conditions
$\psi(s)$	rational function of initial conditions
t_k	discrete time moment
T_v	sampling period
n	degree of the polynomial $a(s)$
m	degree of the polynomial $b(s)$
$\boldsymbol{\varphi}(t_k)$	data vector in continuous-time ELM
$\boldsymbol{\theta}(t_k)$	vector of parameters in continuous-time ELM
q	shifting operator
z, z^{-1}	discrete-time complex variable
$U(z)$	Z-transformation of the input variable
$Y(z)$	Z-transformation of the output variable
$G(z)$	discrete-time transfer function of the system
$a(z)$, $b(z)$	discrete-time polynomials in the transfer function of the system $G(z)$
$e(k)$	random immeasurable component
δ	shifting operator in delta
γ	complex variable in delta
β	optional parameter in delta
$a'(z)$, $b'(z)$	discrete-time polynomials in transfer function of the system $G(z)$ in delta
t'	discrete time for delta
$u_\delta(k)$	input variable in delta
$y_\delta(k)$	output variable in delta

$\boldsymbol{\varphi}_\delta(k)$	data vector in delta ELM
$\boldsymbol{\theta}_\delta(k)$	vector of parameters in delta ELM
$\hat{y}(k)$	estimated output variable
$\varepsilon(k)$	prediction error
$\boldsymbol{\theta}(k)$	estimated vector of parameters
$\boldsymbol{P}(k)$	covariance matrix
$\boldsymbol{L}(k)$	additional vector for identification
$\gamma(k)$	additional constant for identification
$\lambda_0,\lambda_1(k),\lambda_2(k)$	forgetting factors for identification
J	cost function
K	constant
$r(k),\beta(k),\eta(k),\upsilon(k),\kappa(k),\rho_i$	auxiliary constants for identification with directional forgetting
$Q(s)$, $R(s)$	transfer functions of the controller
$W(s)$	transfer functions of the reference signal
$V(s)$	transfer functions of the disturbance
$E(s)$	transfer functions of the control error
$h_w(s),h_v(s)$	numerators of $W(s)$ and $V(s)$
$f_w(s),f_v(s)$	denominators of $W(s)$ and $V(s)$
$p(s),q(s),r(s)$	polynomials in the controller transfer functions $Q(s)$ and $R(s)$
$d(s)$	optional stable polynomial on the right side of Diophantine equations
$\tilde{p}(s)$	modified polynomial $p(s)$
$f(s)$	least common divisor from $f_w(s)$ and $f_v(s)$
$w(t)$	reference signal (wanted value)

$t(s)$	auxiliary polynomial
k_d	constant
s_i	roots of the polynomial $d(s)$
α_i	real part of the root s_i
ω_i	imaginary part of the root s_i
$m(s)$, $n(s)$,$g(s)$	parts of the polynomial $d(s)$
$a^*(s)$,$n^*(s)$	spectral pairs of polynomials $a(s)$ and $n(s)$
μ_{LQ},φ_{LQ}	weighting factors in LQ
$\dot{u}(t)$	difference of the input variable in LQ
J_{LQ}	cost function in LQ
J_{GPC}	const function in GPC
N_u	control horizon
N_1,N_2	minimum and maximum costing horizons
$\delta_u(j)$,$\lambda_u(j)$	weighting sequences in GPC
j	discrete time step
$E_j(z^{-1})$, $F_j(z^{-1})$	polynomials obtained by dividing of 1 by $A(z^{-1})$
d	dead time of the system
e_j,f_j	coefficients of polynomials $E_j(z^{-1})$, $F_j(z^{-1})$
$G_j(z^{-1})$	additional polynomial
g_j	coefficients of the polynomial $G_j(z^{-1})$
$\boldsymbol{G}$,$\boldsymbol{F}$,$\boldsymbol{y}$,$\boldsymbol{u}$	vector forms of the polynomials $G_j(z^{-1})$, $F_j(z^{-1})$ and $y(j)$, $u(j)$
$\boldsymbol{w}$	vector of reference values
$\boldsymbol{H}$,$\boldsymbol{b}$,$\boldsymbol{f}_0$	auxiliary matrixes and vectors

II. PRACTICAL PART

c_A	concentration of the compound A	$[kmol.m^{-3}]$
c_B	concentration of the compound B	$[kmol.m^{-3}]$
T_r	temperature of the reactant	$[K]$
T_c	temperature of the cooling	$[K]$
q_r	volumetric flow rate of the reactant	$[m^3.min^{-1}]$
V_r	volume or reactant	$[m^3]$
k_1, k_2, k_3	reaction rates	$[min^{-1}, min^{-1}.kmol^{-1}]$
k_{01}, k_{02}, k_{03}	pre-exponential factors	$[min^{-1}, min^{-1}.kmol^{-1}]$
T_{r0}	input temperature of the reactant	$[K]$
h_r	reaction heat	$[kJ.min^{-1}.m^{-3}]$
A_r	surface of the cooling jacket	$[m^2]$
U, U_1, U_2	heat transfer coefficients	$[kJ.min^{-1}.m^{-2}.K^{-1}]$
c_{pr}	specific heat capacity of the reactant	$[kJ.kg^{-1}.K^{-1}]$
c_{pc}	specific heat capacity of the coolant	$[kJ.kg^{-1}.K^{-1}]$
m_c	weight of the coolant	$[kg]$
Q_c	heat removal of the cooling liquid	$[kJ.min^{-1}]$
E_1, E_2, E_3	activation energies for reactions	$[kJ.kmol^{-1}]$
h_1, h_2, h_3	enthalpy of reactions	$[kJ.kmol^{-1}]$
n_1	number of pipes in tubular reactor	
$(\cdot)^s$	steady-state values of the state variables	
$(\cdot)_0$	initial-state values of the state variables	
t	time variable	$[s, min]$

z	space variable	$[m]$
$u(t)$	input variables	[%]
$w(t)$	wanted value (reference signal)	$[kmol.m^{-3}, mS]$
$v_{1\text{-}3}(t)$	disturbances	$[\%, K]$
$y_{1\text{-}5}(t)$	output variables	$[kmol.m^{-3}, K, mS]$
S_u,S_y	control quality criteria	[-]
i	step in the computation of S_u and S_y	[-]
N	number of steps in the computation of S_u and S_y	[-]
T_f	time of the simulation	$[s, min]$
α_i	position of the root	[-]
μ_{LQ},φ_{LQ}	weighting factors in LQ	[-]
δ_u,λ_u	weighting sequences in GPC	[-]
v_r, v_c	fluid velocities	$[m.s^{-1}]$
f_r,f_c	constants	$[m^2]$
T_w	temperature of the pipe wall	$[K]$
d_1, d_2, d_3	diameters	$[m]$
$x(t)$	general variable	[-]
h_z	discretization step	$[m]$
L	length of the reactor	$[m]$
N_z	number of parts	[-]

INTRODUCTION

Chemical reactors belong to the most often equipments in the chemical and biochemical industry. Simulation and modelling possibilities rise with the increasing impact of the digital technology and especially with the computer technology which grows exponentially every moment. You can find intelligent control system in every field of the human living, not only industry.

The goal of the work is to apply some of these methods on specific types of chemical reactors like Continuous Stirred Tank Reactors (CSTR) and tubular chemical reactors.

Specific design of the controller is usually preceed by few very important steps. Not every property of the controlled system is known before we start and that is why we perform simulation experiments on the system. There are two main types of the simulation – (1) experiment on the real model and (2) computer simulation. Computer simulation is very often used at present as it has many advantages over an experiment on a real system, which is not feasible and can be dangerous, or time and money demanding.

The first step is system model creation. This model is usually a mathematical model which describes the original process in the best way. Balances inside the reactor are usually used for mathematical model creation. Resulted set of the differential equations is then subjected to the static and dynamic analysis.

The static analysis displays behaviour of the system in the system in the steady-state. This study results in the optimal working point. On the other hand, the dynamic analysis provides step, frequency responses etc. which display dynamic behaviour of the system and they are a base for choosing an external linear model. Numerical mathematics is widely used in the solution of these two analyses.

Many chemical processes have nonlinear properties. There are several methods how to overcome nonlinearity. One approach is choosing the External Linear Model (ELM). If the input variable is a step function, we can call the course of the output variable a “step response”. This step response is then used as a guide to the optimal ELM selection.

The next step after simulation is to look at the problem from the control point of view. Two main control strategies were used in the work – the adaptive control and the generalized predictive control. The adaptive control in this work is based on recursive identification of the ELM of the controlled plant and these parameters are then used for computation of the controller. The second control strategy, the predictive control, is based on calculation of the future values of the input (manipulated) variable which force output variable close to the reference signal (wanted value) and minimize control error in defined prediction horizon.

The work is divided in the five main numbered chapters.

The first chapter gives overview in the research area of the modelling, simulation, identification and control whereas *the second chapter* formulates the main goals of this dissertation.

The section *number three* is focused on the theoretical knowledge about the process from the modelling through the simulation to the control of the process. The last sub-chapter is describes types of chemical reactors used in industry.

The fourth part of the work shows simulation results of the steady-state, dynamic and control analyses for continuous stirred tank reactor and plug-flow reactor and results from the control analyses on the real model of the continuous stirred tank reactor.

The last part is discussion of the obtained results and conclusion of the achieved goals in this work.

Tables, figures and equations are numbered recursively within a chapter and literature is referred to in square brackets.

1 STATE OF ART

It is known that almost all processes in the nature have a nonlinear behaviour. The goal of all researchers in nonlinear theory is to somehow overcome this nonlinearity.

Typical examples of nonlinear systems are chemical processes. One of the most important chemical equipment types is *chemical reactor*. *A chemical reactor* is a vessel or pipe which is used for the production of chemicals used in chemical, biochemical, drug and other industries through a specific reaction inside. Reactors should be divided in several ways – by the chemical reaction inside the reactor [1], by the kinetics [2] and [3] etc. The division from the construction point of view ([4], [2]) is one of the most common. We can come across a *batch*, *semi-batch reactor* or *a continuous stirred tank reactor* (CSTR) or *series of CSTR's*. These reactors belong to the class of tank-reactor equipment, while the *tubular chemical reactor* is a typical member of the pipe-reactor [5].

The starting period for the investigation of the chemical processes can be set the beginning of the 1940s but the real starting point of the process control theory was in the 1970s, when the energy costs had a high importance [6] and the increasing development of the computer technology provided a better verification of theoretical knowledge.

As written above, expansion of the process control theory is connected with the improvements in the computer field but computer programs have been mainly used in the last step of the simulation or control procedure. *The modelling* could be assigned as a starting point of the simulation [7], [8] and [9]. *The model* of the process is a simplified version of the real system and includes all variables and relations of the system which are important for the investigation [10]. The mathematical and physical models are two main types of models used nowadays.

The mathematical model is a kind of abstract representation of the process which uses input, state or output variables, relations between these variables collected in the set of mathematical equations – [4], [6]. The mathematical model is usually a set of linear or nonlinear, normal or differential equations. A very important step in the mathematical model creation is the decision which quantities are constant and introduction of

simplifications. Processes generally, not only chemical processes, are often nonlinear and mathematical description of all quantities and relations inside the process can lead to a very intricate set of equations. Simplifications should reduce this complexity and ensure mathematical solvability.

Mathematical solution of a mathematical model depends on the type of the model. A linear or nonlinear set of ordinary equations is the simplest example of the solution – the simple *Gauss elimination method*, *Cramer's rule*, *Inverse matrix* or *Least-squares method* could be used for numerical solution of this set of linear equations [11], [12]. On the other hand, the *Simple iterative* method and its modifications like *Newton method etc.* [13] are usually used for nonlinear equations [11].

Unfortunately, most of the systems in the nature, not only in chemical industry, have nonlinear properties and they are described by the a of *ordinary differential equations* (ODE) for systems with lumped parameters or *partial differential equations* (PDE) for systems with distributed parameters [14]. The difficulty of finding the solution increases with the nonlinearity and degree of the differential equations. A lot of numerical solution methods have been developed, especially for the ODE, such as *Euler's method* or *Taylor's method* [15]. *Runge-Kutta's methods* are very popular because of their simplicity and easy programmability [16]. Although this method was developed by German mathematicians *Carle David Tolmé Runge* (1856 - 1927) and *Martin Wilhelm Kutta* (1867 - 1944) at the very beginning of the 20th century, it is still very often used in numerical mathematics for the solution of ODE. This method was being improved during the whole 20th century, which resulted in Runge-Kutta's modifications, like the fourth order Runge-Kutta's method, Adaptive Runge-Kutta methods (*Runge-Kutta-Fehlberg Method*) [15] etc. An other multistep method for numerical solution of ODE is the Predictor-Corrector method [17]. The solution of PDE is more complicated because of the presence of usually two types of derivatives – derivatives with respect to time and with respect to the space variable. The set of PDE should be numerically solvable for example by the *Bäcklund transformation*, *Green's function*, *separation of variables* or *finite differences method* [18]. It is clear that the solution of the PDE is very complex; one way how to overcome the

derivative with respect to the space variable is to replace this derivative by difference in time related to the time step and the set of PDE is then transformed to the set of ODE [19].

An indivisible part of the simulation study is steady-state analysis which discovers the behaviour of the system in steady-state, i.e. in the time close to infinity. Mathematically it means that derivatives with respect to time variable are equal to zero. The set of ODE is transformed to the set of linear or nonlinear equations and the set of PDE is now rewritten to the set of ODE with only one derivative with respect to the space variable [19]. The resulted steady-state characteristics show mainly linear or nonlinear behaviour of the system and they can be used for choosing the optimal working point. The optimal working point means the value of the input (manipulated) variable for which the steady-state value of the output variable reaches the maximum.

Once we know the static and dynamic behaviour of the process, we can continue with the design of the controller. In the nearly 1940^{th} a lot of control techniques based on the static and dynamic characteristics of the system were introduced – e.g. design of the controller based on the step response of the system or Ziegler-Nichols method, Tyreus-Luyben [20], which results in a Proportional (usually denoted as *P*), Proportional-Integral (*PI*), Proportional-Derivative (*PD*) or Proportional-Integral-Derivative (*PID*) controller. A disadvantage of these approaches is that the resulting controller has fixed parameters and structure, which is not very suitable for nonlinear systems or systems with negative control properties like time-delay systems, non-minimum phase systems of systems with changing the sign of gain.

One way how to overcome the problems with nonlinearity or the negative control properties in general is the use of the *Adaptive control* [21], [22] and [23]. As can been seen from the term this approach is based on the quality of real organisms which can change behaviour according to environmental conditions. This process is usually called "*adaptation*".

The beginning of adaptive control dates back to over fifty years ago, but a great impact of the adaptive controllers appeared after 1989 with the publishing of the book by Astrom [21] (this was reorganized and some new chapters were added to the second

edition in 1994 [22]). In literature the adaptive controller is tightly connected with the *self-tuning controller*. The self-tuning technique is subset of the adaptive control. The self-tuning controller adapts its parameters at the beginning of the control or in some period before the control starts and the structure is then fixed in contrast to pure adaptive controller which recomputes and changes parameters or structure of the controller in every step during control [24].

The adaptive approach in this work is based on choosing the *external linear model* (ELM) as a mathematical representation of the originally nonlinear process whose parameters are identified recursively during the control. The parameters of the controller are recomputed recursively too, with the dependence on the identified parameters of the ELM. The structure of this ELM could be derived from the dynamic behaviour of the system and is usually represented by the transfer function.

The transfer function of the ELM can be defined in the *continuous* or *discrete* time domain [20]. The *continuous-time* (*CT*) *model* [25] represents a system in continuous time which can cause computational problems because the derivatives of the input and the output variables used in the identification part are immeasurable. This inconvenience can be overcome using differential filters [26]. On the other hand, *discrete models* have no problems with measurements of the input and output variables because their values are measured only in defined times distanced by the sampling period. The choice of the sampling period can be a problem because a small sampling period means that the computer does not have enough time to do all computation, a big sampling period, on the other hand, can cause large dynamic changes inside the system which results in problems for the controller.

A special type of the discrete models is *Delta models* (*δ-models*) [27], [28]. Although they belong to the class of discrete models, the parameters are related to the sampling period, and it was shown in [29] that these parameters are similar to the continuous ones for a small value of the sampling period.

As written above, the parameters of the ELM are identified recursively during control from the values of the input and output variables. The recursive identification is

usually connected with the *Least-squares method,* which is rather old but on the other hand it is simple and has still sufficient results. Several modifications of the *Recursive Least-squares* (RLS) method have been developed, like RLS with exponential forgetting [30] and [31], directional forgetting [32], adaptive directional forgetting [33] or the method with modification of the covariance matrix [34].

An inseparable step in the identification is the design of identification model. Identification models are divided from the error point of view into equation error models (ARX, ARMAX, etc.) and output error models (OE, Box-Jenkins, etc.) [30]. The *auto-regressive exogenous* (ARX) model is the most common used scheme because it is simple and the output variable is a simple linear function of the measured data [35]. On the other hand, the *auto-regressive moving average exogenous* (ARMAX) model consists in the description of a prediction error and the computation of the output variable is made by pseudolinear regression [36] because this output variable is a nonlinear function of the measured data.

The mathematical description of the process and the controller by polynomials is an algebraic method often used in the synthesis of the controller [37], [38]. This, so called *polynomial synthesis,* works in the ring of polynomials and is derived from the input-output model of the system or controller. The polynomial approach has some good properties, such as it fullfiling basic control requirements (stability, properness) and it provides not only the structure of the controller but also the relations for the computing of the controller's parameters. And last but not least, this method is easily programmable.

One of the demands on the controller is that it should be tunable. The polynomial synthesis in this work results in solving of the Diophantine equation, or the set of equations, which has an optional stable polynomial on the right side of the equation and the choice of parameters of this polynomial affects the control response. The *Pole-placement* [38] (in some literature called the *Pole-assignment method*) is one of the methods used in this case. The placement of roots is sometimes difficult and there is no rule how to choose the right pole. It is good to connect the stable polynomial with the parameters of the controlled system or ELM, respectively for example with the spectral factorization [39]. *The Linear Quadratic* (*LQ*) approach is the second possible way for designing the stable polynomial

on the right side of the Diophantine equation [26]. The LQ is based on the minimizing of the cost function.

Another possibility how to influence the quality of the control is to use different control configurations. The first configuration has a controller in the feedback part and is called a *one-degree-of-freedom* (*1DOF*) *control configuration* [40]. It was proofed in [41] that a two-degree-of-freedom configuration (2DOF), which has one part of the controller in the feedback and the other in the feedforward part, has better control results, especially at the beginning of the control, than the basic 1DOF configuration.

The simulation results for different types of nonlinear models [26], [42] and [43] have shown that the adaptive controllers connected with polynomial methods can be applied on systems with negative control properties, such as instability, non-minimum phase or on systems with transport delays because they fulfill basic control requirements, such as stability, properness, asymptotic tracking of the reference or disturbance attenuation.

The last years of the 20th century and the beginning of the 21st century are in token of developing "modern control methods" like Adaptive control [21], [22], Predictive control [44], [45], [46] and [47], Model predictive control [48], [49] and [50], Robust control [51] or application of neural networks and Artificial Intelligence [52].

2 DISSERTATION GOALS

The aim of this dissertation is to apply and verify some novel control methods to chemical reactors. Verifications are done by simulation on a mathematical model in the computer and some methods are then applied on a real chemical reactor.

It is impossible to include all modern control methods so in this work I choose several of them which have preferably general description, are easily programmable and do not depend on the computation power of computer.

The goals of the present work can be summarized in the following points:

1. To perform static and dynamic analyses of different types of stirred reactors and tubular reactor.
2. To prepare different modern control algorithms to control these chemical reactors and verify these algorithms by simulation.
3. To verify the proposed controllers from the simulation part on a real model of the continuous stirred tank reactor (CSTR).

3 THEORETICAL FRAMEWORK

The theoretical part is mainly focused on the description of the theoretical background of the modelling, simulation, static and dynamic analyses, adaptive and predictive control.

3.1 Modeling and Simulation

It is common for the industrial processes that they are considered as "black boxes" which means that we do not know internal structure of the system, but only input-output measurements are at our disposal. Simulation is one way how we can overcome this internal uncertainty. From the input-output measurements we can obtain properties of the system in the mathematical terms like differential equations, transfer functions, step or impulse functions etc. [20]

3.1.1 Types of Systems

It will be good to describe basic types of systems before we start with the modelling, identification and simulation of them.

There are several types of systems. The first division is into the *linear* and *nonlinear systems*. Relations between variables inside the model are described by the linear functions while nonlinear models have the relations from the range of nonlinear functions.

Systems where state variables are position independent are called *systems with lumped parameters*; unlike *systems with distributed parameters* where state variables are functions of time and space variable.

Variables in the *continuous-time systems* are defined in the continuous time interval unlike in *discrete-time systems* where one of the quantities is specified in the discrete time.

Deterministic systems are those whose actual output is derived from the previous state and the input variable while the state of the system should be defined only with some

probability in *stochastic systems*. Uncertainty of these systems is caused as an effect of the random signals in the output of the system.

Next divisions are *stationary (time-invariant) systems* where variables do not depend on time unlike in *nonstationary (time-variant) systems*. The *single-input single-output* (SISO) system has only one input and one output whereas systems with more than one signal on the input or output like single-input multiple-output (SIMO) systems, multiple-input single-output (MISO) systems and multiple-input multiple-output (MIMO) systems belongs to the class of *multivariable systems*.

3.1.2 Modelling

There are two main types of the models – *physical* (*real*) *models* and *abstract models*. The real model is represented by the copy of the system, usually small or similar to the original one. On the other hand, the mathematical model is usually used as an abstract model of the system.

As is written above, modelling and simulation are the first steps in the design of the controller. Two approaches should be used in the modelling part. The first method collects measurement results of input and output variables. The resulted model is called *input-output model* and the method is named *empiric approach*. Disadvantage of this model is that it describes only relation between the input and the output variable and does not give any information of the system's structure.

Process is usually described by various types of quantities like temperature, pressure, flow rate, concentration etc. which describe the process from the mathematical point of view. These quantities are called *state variables* and relations between them are used for the second method – *the analytic approach*. The resulted *analytic* (or more common used "*mathematical*") *model* describes these inner variables, relations between them and we can imagine it as a set of linear, nonlinear, ordinary differential equations (ODE) and a set of partial differential equations (PDE).

The mathematical model is only abstract approximation of the real system which is very complex or partly misunderstood [4]. Thus models do not strictly describe all the properties and relations inside the system, but pick up the most important ones and introduce constants and simplifications. It is required that mathematical model describe real system in the proper way and moreover it is in the simplest one from the range of available models. To find compromise between these two claims is the most important part of modelling.

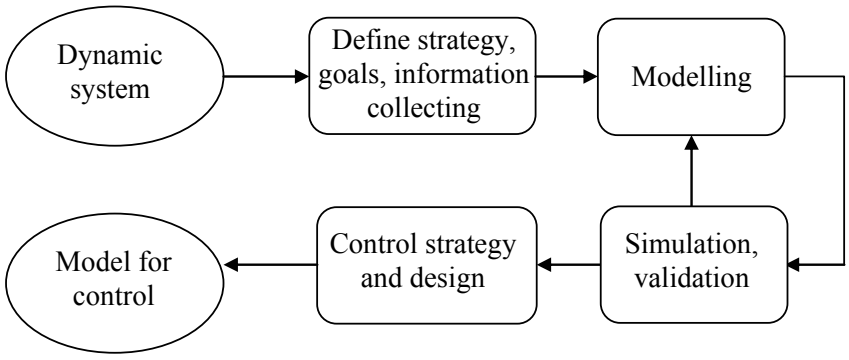


Figure 3.1 General modelling procedure

Figure 3.1 shows the main stages in the modelling procedure. First we start with the definition of goals and requirements and general description of the system, usually dynamical system.

The next step is connected with collecting all available knowledge of the system. This work needs deeper knowledge about the background of the system, its behaviour, reactions and chemical process inside of it etc. It is common that this work means the exchange of the experience with the industry.

The most important relations are then put together in mathematical model which is then simulated by the computer. Validity of the model is checked by the comparison with the results of the experiments on the real model. If the results agree sufficiently we can use this model for mathematical simulation. It is common that convenience of the model is revised in predefined intervals.

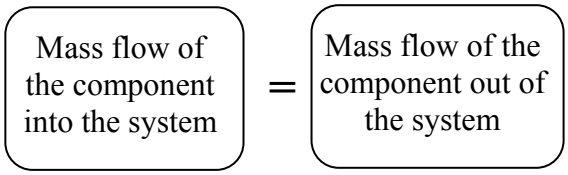
The last steps are related to choosing of the control strategy and design of the controller.

MATHEMATICAL BALANCES

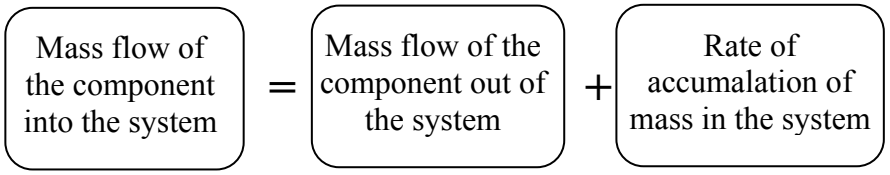
The mathematical model of the system usually comes from *mathematical balances* inside the reactor. They include kinetic equations for rates of the chemical reactions, heat rates, heat transfers and equations which represents property changes. The resulted model should be the simplest one but unfortunately it is very complex. In this case we must introduce assumptions which decrease complexity of the model but preserve the most important relations.

Material balance

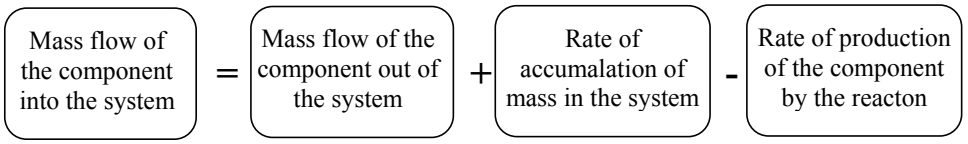
Material balance in the steady-state can be generally described in the word form as



However, most of the variables vary in time and steady-state balance is not suitable. We can introduce dynamic material balance which contains changes with respect to time in the form of accumulation

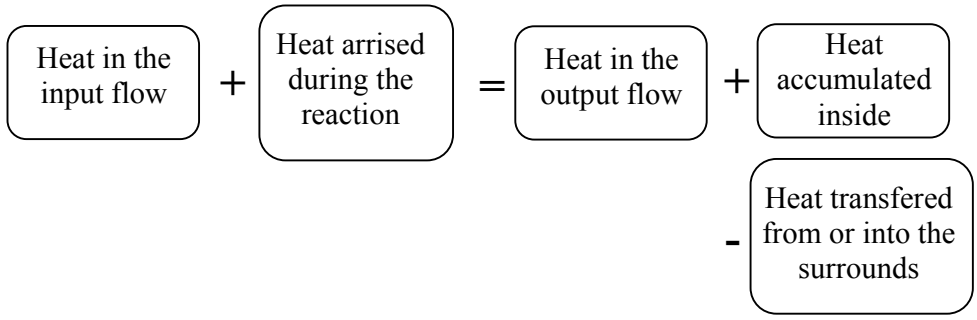


Some of the processes include chemical reactions. Material balance is in this case



Heat balance

Heat balance is usually the second type of balances used in modelling procedure. Temperature changes are usually caused by the reaction heat or cooling. This must be mentioned in case where heat changes inside the system are significant. The word form of this balance is



Mathematical description

The *nonlinear time-invariant systems with lumped parameters* are generally described by the set:

$$\begin{aligned} \dot{\boldsymbol{x}}(t) &= \boldsymbol{f}\left[\boldsymbol{x}(t), \boldsymbol{u}(t)\right] \\ \boldsymbol{y}(t) &= \boldsymbol{g}\left[\boldsymbol{x}(t), \boldsymbol{u}(t)\right] \end{aligned} \tag{3.1}$$

where $\boldsymbol{x}(t) = [x_1(t), x_2(t), \ldots x_n(t)]^T$ is the state vector, $\boldsymbol{u}(t) = [u_1(t), u_2(t), \ldots u_m(t)]^T$ denotes the input vector, $\boldsymbol{f} = [f_1, f_2, \ldots f_n]^T$ and $\boldsymbol{g} = [g_1, g_2, \ldots g_n]^T$ are nonlinear vector functions.

Once the mathematical model is constructed, it is important to define its *conditions*. Each state variable needs as many conditions as is the highest order of the derivative related to the independent variable in differential equations.

The system described by the set (3.1) has *initial condition*

$$\boldsymbol{x}(0) = \boldsymbol{x}_0^s \tag{3.2}$$

which are obtained from the steady-state analysis described later.

On the other hand, one part of *systems with distributed parameters* with ideal plug-flow inside have the mathematical model in the form of PDE. The equation which describes one of the state variables could be

$$\frac{\partial x(z,t)}{\partial t} - a\frac{\partial^2 x(z,t)}{\partial z^2} + v\frac{\partial x(z,t)}{\partial z} = f\left[x(z,t), u(z,t)\right] \tag{3.3}$$

where z is space variable, t denotes time, a and v are constants and f is nonlinear function. In this case we need not only *initial conditions* but *boundary conditions* too, in this case:

$$x(0,t) = u^0(t) \text{ or } x(L,t) = u^L(t) \tag{3.4}$$

where $u^0(t)$ and $u^L(t)$ are called boundary input variables.

The second part with the squared derivative with respect to space variable ($\partial^2 x(t,z)/\partial z^2$) usually deal with longitudinal diffusion, heat conduction or longitudinal interfusion etc. and this part is often neglected due to small values of elements of the constant a.

The boundary conditions can be written as

$$\alpha_1\frac{\partial x}{\partial z} + \beta_1(u^0 - x)\Big|_{z=0} = 0\,,\ \alpha_2\frac{\partial x}{\partial z} - \beta_2(u^L - x)\Big|_{z=L} = 0 \tag{3.5}$$

where $\alpha, \beta \geq 0$ are constants and $u^0(t)$, $u^L(t)$ are again boundary input variables.

If we set $\alpha_1 = \alpha_2 = 0$, eq. (3.5) is called *the first type of boundary condition*. Furthermore, $\beta_1 = \beta_2 = 0$ results in *the second type of boundary condition* and for non-zero α and β we obtain *the third type of boundary condition*. *The mixed boundary condition* is obtained in the case where we have different types of conditions on the right and left side of the reactor. Boundary conditions must be chosen according to physical properties of the process.

The *initial condition* for both cases is

$$x(z,0) = x^s(z) \tag{3.6}$$

where $x^s(z)$ comes from steady-state, i.e. for ODE where derivations are only with respect to space variable z and all boundary and input variables are in steady-state too.

3.1.3 Steady-state Analysis

Analyses inside the reactor are the next step after the developing of the mathematical model, initial and boundary conditions. There were used steady-state and dynamic analysis to obtain information about the type and behaviour of the system. Steady-state analysis results in optimal working point while the product of dynamic analysis could be step, frequency etc. responses.

Steady-state analysis for stable systems involves computing values of state variables in time $t \rightarrow \infty$, when changes of these variables are equal to zero. That means that all equations which consist of derivations with respect to zero have these derivations equal to zero, i.e.

$$\frac{d(\cdot)}{dt} = 0 \tag{3.7}$$

There are many methods for solving of this problem. If the system is linear, the set of differential equations can be rewritten to the set of linear equations which can be solved by general, well known methods like matrix-inversion, Gauss elimination etc. or with the use of some types of iterative methods. However, the most of the processes are nonlinear which leads us to the set of nonlinear equations. Despite the fact that there is a possibility of the analytical solution, iterative methods are used more often.

The other possibility is *the simple iterative method* [6] which is often used for defined form of the equations. This method leads to the exact solution for appropriate

choice of initial iteration and for the fulfilled convergence condition. Its advantage is that it does not need special modifications and side calculations according to other iterative methods like Newton's method etc. Although this method converges slower than Newton's method, this disadvantage is unimportant nowadays, when the speed of computers is very high. This method will be used for solving of a steady-state.

The simple iterative method

Consider nonlinear system in the for of state equation similar as in Equation (3.1)

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}\left[\boldsymbol{x}(t), \boldsymbol{u}(t)\right] \tag{3.8}$$

with initial condition

$$\boldsymbol{x}(0) = \boldsymbol{x}^s \tag{3.9}$$

The vector of input variables is

$$\boldsymbol{x}^s = \left[x_1^s, x_2^s, \ldots x_n^s\right]^T \tag{3.10}$$

Components of this vector are unknown and they could be computed by solving of equations of the model in steady-state:

$$\boldsymbol{f} = \left(\boldsymbol{x}^s, \boldsymbol{u}^s\right) = 0 \tag{3.11}$$

where $\boldsymbol{u}^s = [u_1{}^s, u_2{}^s, \ldots u_{\mathrm{m}}{}^s]^T$ is vector of assigned (known) input variables which comes from basic steady-state. Unknown variables in the equation (3.11) are components of the state vector $\boldsymbol{x}^s$, which creates n state variables in basic steady-state. This basic steady-state is called *working point of the system* and surrounding of this point is used for dynamic analysis of the system (3.8).

Computation of the initial conditions $\boldsymbol{x}^s$ is for nonlinear system important not only for computation of the dynamics but also it is used for creating of a linearized

mathematical model of the process in working point. It is known that parameters of this model depend on values of state variables in the working point.

Equation (3.11) can be now rewritten to

$$\boldsymbol{f}(\boldsymbol{x}) = 0 \tag{3.12}$$

for unknown values of x_i for $i = 1,2,\ldots n$.

Next step in the solution is following. The equivalent set of equations to the set (3.12) is

$$\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{x}) \tag{3.13}$$

where φ is nonlinear vector function $\boldsymbol{\varphi} = [\varphi_1, \varphi_2, \ldots \varphi_n]^T$ and which leads to iterative equation in the form of

$$\boldsymbol{x}^{k+1} = \boldsymbol{\varphi}\left(\boldsymbol{x}^k\right) \text{ for } k = 0,1, \ldots \tag{3.14}$$

The iterative method leads to the exact solution only if it converges. *The convergence condition* of the iterative process (3.14) then can be formulated as follows:

Let the vector function φ is defined in the closed convex region $D \subset \Re^n$ and if $\boldsymbol{x} \in D$ so $\boldsymbol{\varphi} \in D$ too. Moreover, let functions φ has continuous partial differential derivations of all variables $x_1 \div x_n$ in the region D, then there exists matrix

$$\boldsymbol{\varphi}'(\boldsymbol{x}) = \frac{d\boldsymbol{\varphi}}{d\boldsymbol{x}} = \begin{pmatrix} \frac{d\varphi_1}{dx_1} & \frac{d\varphi_1}{dx_2} & \cdots & \frac{d\varphi_1}{dx_n} \\ \frac{d\varphi_2}{dx_1} & \frac{d\varphi_2}{dx_2} & \cdots & \frac{d\varphi_2}{dx_n} \\ \vdots & & \ddots & \\ \frac{d\varphi_n}{dx_1} & \frac{d\varphi_n}{dx_2} & \cdots & \frac{d\varphi_n}{dx_n} \end{pmatrix} \tag{3.15}$$

If matrix (3.15) complete condition $\|\boldsymbol{\varphi}'(\boldsymbol{x})\| < 1$ for any $\boldsymbol{x} \in D$, there are only one solution $\boldsymbol{x}^* \in D$ of the equation (3.14).

There could be of course thousands of iterations during the computation but from practical point of view is convenient to stop the computation in the case that difference between values of actual and previous iteration is sufficiently small, i.e. condition

$$\left\| \boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)} \right\| < \varepsilon_{ss} \tag{3.16}$$

is fulfilled for accuracy $\varepsilon_{ss} > 0$, value of which depends on supposed absolute dimension of computed variables.

It is important to introduce following remarks in addition to the previous conditions:

- This method can be used for cases where steady-state model (3.11) includes linear part besides nonlinear part. Linear part is necessary for creation of a equivalent set (3.13). The iterative equation of the heat transfer balance includes both linear part for heat transfer and nonlinear part computed from Arrhenius law.
- The input iteration should be selected from the convergence region of the iterative process. The temperature inside of the reactor is supposed to by higher than the temperature of the input flow. Therefore it is convenient to set the input iteration equal to this temperature.

3.1.4 Dynamic Analysis

Dynamic analysis is usually the next step after the steady-state analysis. Dynamic analysis for systems with lumped parameters is mainly focused on the numerical solving of the set of ODE described as (3.8). There are a lot of methods which can be used for numerical solving of this problem. General division is into the two main groups – one-step and multi-step methods.

We supposed the general differential equation be in the form of (3.1)

$$\boldsymbol{y}(t) = \boldsymbol{g}\left[\boldsymbol{x}(t), \boldsymbol{u}(t)\right] \tag{3.17}$$

with the initial condition

$$y(t_0) = y_0 \tag{3.18}$$

which is called Cauchy Problem [30].

Although there are a lot of methods for solution of ODE, the popular Runge-Kutta's standard method was used in this work. This method is very often used in the praxis because of its simplicity. Runge-Kutta's methods belong to the class of high-order methods, they can be used for computation of the initial values or for the final result and they are easily programmable. The fourth-order Runge Kutta's method is one of the most used types [6] and [12]. This method uses first four parts of the Taylor's series:

$$y(k+1) = y(k) + \frac{1}{6} \cdot \left(g_1 + 2g_2 + 2g_3 + g_4\right) \tag{3.19}$$

where coefficients $g_{1\text{-}4}$ are computed from:

$$\begin{aligned}
g_1 &= h_i \cdot f\left(x_n, y(x_n)\right) \\
g_2 &= h_i \cdot f\left(x_n + \frac{h_i}{2}, y(x_n) + \frac{g_1}{2}\right) \\
g_3 &= h_i \cdot f\left(x_n + \frac{h_i}{2}, y(x_n) + \frac{g_2}{2}\right) \\
g_4 &= h_i \cdot f\left(x_n + h_i, y(x_n) + g_3\right)
\end{aligned} \tag{3.20}$$

The Runge-Kutta's methods are in some cases build-in functions in mathematical softwares. For example in MATLAB, which is used for simulation in this work, are Runge-Kutta's methods in functions `ode23` (the second order Runge-Kutta formula) or `ode45` (the fourth order Runge-Kutta's formula described above) [53]. One of advantages of these methods is that they have flexible integration step h_i, which recomputes every step

according to the actual computation error. The standart Runge-Kutta method has a several modifications like *Runge-Kutta-Fehlberk* method, *Runge-Kutta-Nyström* method etc [54].

As it is mentioned above, systems with distributed parameters are usually described by the set of PDE. Direct numerical solving of the PDEs is very complex. Some PDE can be solved with the use of *Bäcklund transformation*, *Green's function*, *separation of variables* or some numerical methods such as *finite elements*. The method of finite differences was used in this work. This method transforms the set of PDE to the set of ODE. This can be done by replacing the variables with respect to the axial variable z by the first back or forward difference [19]:

$$\left.\frac{dy}{dz}\right|_{z=z_i} \approx \frac{y(i)-y(i-1)}{h_z}, \text{ for } i = 1,2,\ldots n \tag{3.21}$$

$$\left.\frac{dy}{dz}\right|_{z=z_i} \approx \frac{y(j+1)-y(j)}{h_z}, \text{ for } j = n\text{-}1, n\text{-}2 \ldots, 1 \tag{3.22}$$

where i, j are indexes, n is number of pieces and h_z is discretization step.

3.2 Identification and Control

Most processes in the nature, not only in chemical industry have nonlinear properties and the use of classical controllers with fixed parameters could result in non-optimal control because of changing parameters of the system.

The use of the “modern” control methods is one way how to overcome this problem. The adaptive and the predictive control were used as a control approaches in this work.

3.2.1 Adaptive Control

The basic idea of adaptive control is that parameters or the structure of the controller are adapted to parameters of the controlled plant according to the selected

criterion [33]. Adaptation can be done for example by the modification of the controller's parameters by the change of the controller's structure or by generating an appropriate input signal, which is called "adaptation by the input signal".

In some references the adaptive system is called *self-tuning system* which is formally subset of the adaptive systems. As written in [24], an adaptive controller is a system with continuous (recursive) adaptation of the parameters while a self-tuning controller adapts parameters only at the beginning of the control and the computation mechanism is switched off.

The adaptive approach in this work is based on choosing an *external linear model* (ELM) of the original nonlinear system whose parameters are recursively identified during the control. Parameters of the resulted continuous controller are recomputed in every step from the estimated parameters of the ELM.

EXTERNAL LINEAR MODELS

The main types of ELM are *continuous-time* (CT) models and *discrete-time* models. Both models are described in detail in the following chapters.

Continuous-time ELM

This approach is based on continuous-time theory described for example in [25]. Models are generally described in the time domain as

$$a(\sigma)y(t) = b(\sigma)u(t) \tag{3.23}$$

where a, b are polynomials of the system, $y(t)$ is output variable, $u(t)$ denotes input variable and σ is the differentiation operator. The initial conditions for Equation (3.23) are

$$\begin{aligned} y^{(i)}(0) &= y_0^{(i)}, \quad i = 0,1,2,\ldots,n \quad \text{for} \quad n = \deg a \\ u^{(j)}(0) &= u_0^{(j)}, \quad j = 0,1,2,\ldots,m \quad \text{for} \quad m = \deg b \end{aligned} \tag{3.24}$$

and Equation (3.23) can be rewritten with the initial conditions equal to zero and with application of the Laplace transformation to the form:

$$a(s)Y(s) = b(s)U(s) + o_1(s) \tag{3.25}$$

where s denotes complex variable, polynomial o_1 includes initial conditions and polynomials $a(s)$ and $b(s)$ are

$$a(s) = \sum_{i=0}^{\deg a} a_i s^i, b(s) = \sum_{j=0}^{\deg b} b_j s^j \tag{3.26}$$

Transfer function $G(s)$ for the initial conditions equal to zero is:

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b(s)}{a(s)} \tag{3.27}$$

Discrete (Z–) ELM

As already said, there is a problem with setting of the polynomial $c(s)$ in Equation (3.31). One solution to this problem is to use of discrete models. These models have, however, one disadvantage; discrete shifting operator q in the general description

$$q \cdot x(k) \triangleq x(k+1) \tag{3.28}$$

is not equivalent to the continuous time operator [55].

Discrete models are used in the cases where the usage of continuous ones is complicated or the realization is impossible. An important variable in the discrete-time models is *sampling period* T_v. The selection of the sampling period is intuitive and there is no general rule for this choice, but one suggestion is to take it from eigt to twelve samples for the active part of the step response. An active part of the step response is a time interval in which the output variable reaches 95% of the steady-state value.

We can generally say that a sufficient number of samples for the description of the step response is a good way for selection of the root. Another limitation is of course the

use of hardware. We cannot take sampling period lower than sampling period of the counters and timers.

The transfer function G in this case is defined as Z-transform of the output variable y to the input variable u

$$G(z)=\frac{Y(z)}{U(z)}=\frac{b(z)}{a(z)}=\frac{b_m z^m+b_{m-1}z^{m-1}+\ldots+b_1 z+b_0}{a_n z^n+a_{n-1}z^{n-1}+\ldots+a_1 z+a_0} \tag{3.29}$$

where $a(z)$ and $b(z)$ are discrete polynomials and $U(z)$ and $Y(z)$ are Z-transform images of the input and output variables.

It is more common that the polynomials are in negative powers of the complex variable z, which means that we divide Equation (3.29) by the highest power of z. The condition of the strict properness says that $\deg a(z) > \deg b(z)$, i.e. $n > m$ and equation (3.29) is divided by z^n:

$$G(z^{-1})=\frac{Y(z^{-1})}{U(z^{-1})}=\frac{b(z^{-1})}{a(z^{-1})}=\frac{b_m z^{m-n}+b_{m-1}z^{m-1-n}+\ldots+b_1 z^{1-n}+b_0 z^{-n}}{a_n+a_{n-1}z^{-1}+\ldots+a_1 z^{1-n}+a_0 z^{-n}} \tag{3.30}$$

This model was mentioned only for the complementarity and it is not used later in the practical part.

ELM PARAMETERS IDENTIFICATION

The use of the discrete model for nonlinear system can cause problems with the sampling period T_v. This sampling period cannot be small because of the stability and the big sampling period is unacceptable because we do not know what will happen with the system during this sample.

The continuous-time ELM with the use of *differential filters* and *δ-models* were used for the identification in this work.

Continuous-time ELM

Equation (3.23) means a problem from the identification point of view because of the derivatives of the input and output variables which are immeasurable. However, these derivations can be replaced by the filtered ones, y_f and u_f, computed from

$$\begin{aligned} c(\sigma)u_f(t) &= u(t) \\ c(\sigma)y_f(t) &= y(t) \end{aligned} \tag{3.31}$$

where $c(\sigma)$ is stable polynomial in σ, which fulfils condition $\deg c(\sigma) \geq \deg a(\sigma)$.

Laplace transformation of Equation (3.31) is then

$$\begin{aligned} c(s)U_f(s) &= U(s) + o_2(s) \\ c(s)Y_f(s) &= Y(s) + o_3(s) \end{aligned} \tag{3.32}$$

where o_2 and o_3 are polynomials which include initial conditions of the filtered variables. Substitution of Equation (3.32) into Equation (3.25) results in

$$Y_f(s) = \frac{b(s)}{a(s)}U_f(s) + \Psi(s) \tag{3.33}$$

and $\Psi(s)$ is rational function in s which contains initial variables of filtered and unfiltered variables.

It is known [26] that dynamics of the filter in Equation (3.31) must be faster than dynamics of the controlled process. The initial choice of polynomial $c(s)$ is connected with the knowledge of the system. One possibility is to choose parameters of $c(s)$ apriory small.

If we take the values of the filtered variables in the discrete time moment $t_k = k \cdot T_v$ for k = 0,1,2,… where T_v is sampling period, the regression vector for deg $a = n$ and deg $b = m$ is

$$\boldsymbol{\varphi}(t_k) = \left[-y_f(t_k), -y_f^{(1)}(t_k), \ldots, -y_f^{(n-1)}(t_k), u_f(t_k), u_f^{(1)}(t_k), \ldots, u_f^{(m)}(t_k), 1\right]^T \tag{3.34}$$

and the vector of parameters is

$$\boldsymbol{\theta}(t_k) = \left[a_0, a_1, \ldots, a_{n-1}, b_0, b_1, \ldots, b_m\right]^T \tag{3.35}$$

The parameters of polynomials $a(s)$ and $b(s)$ are estimated recursively in discrete time moments from equation

$$y_f^{(n)}(t_k) = \boldsymbol{\theta}^T(t_k) \cdot \boldsymbol{\varphi}(t_k) + \Psi(t_k) \tag{3.36}$$

Delta (δ–) ELM

Although the delta operator belongs to the class of discrete models with the operator described in Equation (3.28), it can been seen from

$$\delta = \frac{q-1}{T_v} \tag{3.37}$$

that this operator is related to sampling period T_v and it means that δ-models are close to the continuous ones in d/dt.

Now, a new complex variable in "δ" plane called "γ", which is defined for example in [56] as

$$\gamma = \frac{z-1}{\beta \cdot T_v \cdot z + (1-\beta) \cdot T_v} \tag{3.38}$$

We can obtain an infinite number of δ–models for different values of optional parameter β in Equation (3.38) from the range $0 \le \beta \le 1$.

There are several commonly used δ-models [33]:

$$\text{for } \beta = 0: \gamma = \frac{z-1}{T_v} \; \textit{forward } \delta\textit{-model} \tag{3.39}$$

for $\beta = 1$: $\gamma = \dfrac{z-1}{z \cdot T_v}$ *backward δ-model* (3.40)

for $\beta = 0.5$: $\gamma = \dfrac{2}{T_v}\dfrac{z-1}{z+1}$ *Tustin's δ-model* (3.41)

The forward δ-model described by Equation (3.39) is dealt with in this work. If we have general output function $y(t)$, the approximation of its first derivation by the first difference is $\delta y(t)$ and the relation between differentiation operator σ and δ-operator is [43]

$$\lim_{T_v \to 0} \delta = \sigma \tag{3.42}$$

and the continuous model (3.23) must be rewritten to the form

$$a'(\delta)\, y(t') = b'(\delta)\, u(t') \tag{3.43}$$

where polynomials $a'(\delta), b'(\delta)$ are discrete polynomials and their coefficients are different from those of the CT model $a(s)$ and $b(s)$. Time t' is discrete time.

Now we can introduce substitution $t' = k - n$ for $k \geq n$ and Equation (3.43) then will be

$$\begin{aligned} \delta^n y(k-n) = b'_m \delta^m u(k-n) + \ldots + b'_1 \delta u(k-n) + b'_0 u(k-n) - \\ -a'_{n-1} \delta^{n-1} y(k-n) - \ldots - a'_1 \delta y(k-n) - a'_0 y(k-n) \end{aligned} \tag{3.44}$$

Individual elements are

$$\delta^i y(k-n) = \sum_{j=0}^{i} \frac{(-1)^j}{T_v^i} \binom{i}{j} y(k-n+i-j), \text{ for } i = 0,1,\ldots, n \tag{3.45}$$

$$\delta^l u(k-n) = \sum_{j=0}^{l} \frac{(-1)^j}{T_v^l} \binom{l}{j} u(k-n+l-j), \text{ for } l = 0,1,\ldots, m \tag{3.46}$$

The individual parts in Equation (3.44) can be written as

$$\begin{aligned} y_\delta(k) &= \delta^n y(k-n), & u_\delta(k-n+m) &= \delta^m u(k-n), \\ y_\delta(k-1) &= \delta^{n-1} y(k-n), & u_\delta(k-n+m-1) &= \delta^{m-1} u(k-n), \\ &\vdots & &\vdots \\ y_\delta(k-n+1) &= \delta y(k-n) & u_\delta(k-n+1) &= \delta u(k-n), \\ y_\delta(k-n) &= y(k-n) & u_\delta(k-n) &= u(k-n) \end{aligned} \tag{3.47}$$

and the regression vector is

$$\begin{aligned} \boldsymbol{\varphi}_\delta(k-1) = \big[& -y_\delta(k-1), \ldots, -y_\delta(k-n+1), -y_\delta(k-n), \\ & u_\delta(k+m-n), u_\delta\left(k+m-1-n\right), \ldots, u_\delta(k-n+1), u_\delta(k-n) \big]^T \end{aligned} \tag{3.48}$$

The vector of parameters

$$\boldsymbol{\theta}_\delta\left(k\right) = \left[a'_{n-1}, \ldots, a'_1, a'_0, b'_m, b'_{m-1}, \ldots, b'_1, b'_0 \right]^T \tag{3.49}$$

is then computed from the differential equation

$$y_\delta\left(k\right) = \boldsymbol{\theta}_\delta^T\left(k\right) \cdot \boldsymbol{\varphi}_\delta\left(k-1\right) + e\left(k\right) \tag{3.50}$$

where $e(k)$ is again a general random immeasurable component.

It was proofed for example in [29] that estimated parameters of the δ-model are very close to the CT ones for small values of the sampling period, T_v.

ARX identification model (Auto-Regressive eXogenous)

The identification models can be generally divided into two main groups [30] – *equation error models* (ARX, ARMAX etc.) and *output error models* (OE, Box-Jenkins, FIR etc.). In this work is used ARX model for the identification although the difference between ARX and ARMAX model was verified for example in [63].

If we consider general linear difference equation

$$y(k)+a_1y(k-1)+\ldots+a_ny(k-n)=b_0u(k)+b_1u(k-1)+\ldots+b_mu(k-m)+e(k) \qquad (3.51)$$

where coefficients $a_{1\text{-}n}$ and $b_{0\text{-}m}$ are parameters of the ELM estimated from the identification and n = deg a, m = deg b, $u(t)$ is a input variable and $e(t)$ is stochastic part, for example the effect of immeasurable disturbances. Equation (3.51) can be rewritten as a relation for the estimated output variable $\hat{y}(t)$ in each step

$$\hat{y}(k)=-a_1y(k-1)-\ldots-a_ny_n(k-n)+b_0u(k)+b_1u(k-1)+\ldots+b_mu(k-m)+e(k) \qquad (3.52)$$

and if we introduce general vector of parameters $\boldsymbol{\theta}$ and data vector $\boldsymbol{\phi}$

$$\begin{aligned}\boldsymbol{\theta}&=\left[a_1,\ldots,a_{n_a},b_0,\ldots,b_{n_b}\right]^T\\ \boldsymbol{\varphi}(k)&=\left[-y(k-1),\ldots,-y(k-n),u(k),u(k-1),\ldots,u(k-m)\right]^T\end{aligned} \qquad (3.53)$$

the difference equation (3.51) can be rewritten to vector form:

$$\hat{y}(k)=\boldsymbol{\theta}^T\cdot\boldsymbol{\varphi}(k)+e(k) \qquad (3.54)$$

The ARX model is very often used because the data vector consists only of variables which can be directly measured and there is no need to reconstruct them. The deterministic part can be optional, the estimated output variable is linear function of the measured data and a linear regression can be used for parameter estimation [35].

Recursive Least Squares (RLS) Method and Modifications

The RLS method is often used at adaptive control for on-line identification of the system's parameters. Parameters are recomputed recursively in time – if we know the estimated parameters in the previous step $\hat{\boldsymbol{\theta}}(k-1)$, new estimation $\hat{\boldsymbol{\theta}}(k)$ is obtained by the modification of $\hat{\boldsymbol{\theta}}(k-1)$. One big advantage of RLS methods is that they do not need

to store all data, which is good for the computer memory. They can be easily modified for e.g. changing data in time.

The RLS method can be formally expressed by the following set of equations:

$$\varepsilon(k) = y(k) - \boldsymbol{\varphi}^T(k) \cdot \hat{\boldsymbol{\theta}}(k-1) \tag{3.55}$$

$$\gamma(k) = \left[1 + \boldsymbol{\varphi}^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k)\right]^{-1} \tag{3.56}$$

$$\boldsymbol{L}(k) = \gamma(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k) \tag{3.57}$$

$$\mathbf{P}(k) = \mathbf{P}(k-1) - \gamma(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k) \cdot \boldsymbol{\varphi}^T(k) \cdot \mathbf{P}(k-1) \tag{3.58}$$

$$\hat{\boldsymbol{\theta}}(k) = \hat{\boldsymbol{\theta}}(k-1) + \boldsymbol{L}(k)\varepsilon(k) \tag{3.59}$$

where ε is prediction error and **P** is covariance matrix.

The standard RLS can be modified with the use of the forgetting factor. As shown in [30], covariance matrix is updated by equation

$$\mathbf{P}^{-1}(k) = \mathbf{P}^{-1}(k-1) + \boldsymbol{\varphi}(k) \cdot \boldsymbol{\varphi}^T(k) \tag{3.60}$$

which can be generalized to

$$\mathbf{P}^{-1}(k) = \lambda_1(k-1) \cdot \mathbf{P}^{-1}(k-1) + \lambda_2(k-1) \cdot \boldsymbol{\varphi}(k) \cdot \boldsymbol{\varphi}^T(k) \tag{3.61}$$

where λ_1 and λ_2 are factors which affect covariance matrix **P**. These factors are from the range of $0 < \lambda_1 \leq 1$, $0 < \lambda_2 \leq 2$ and have an opposite effect – λ_1 increases covariance matrix **P** whereas λ_2 decreases it.

Recursive relation (3.58) for computing of covariance matrix **P** is then modified to the form

$$\mathbf{P}(k)=\frac{1}{\lambda_1(k-1)}\left[\mathbf{P}(k-1)-\frac{\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}(k)\cdot\boldsymbol{\varphi}^T(k)\cdot\mathbf{P}(k-1)}{\frac{\lambda_1(k-1)}{\lambda_2(k-1)}+\boldsymbol{\varphi}^T(k)\cdot\mathbf{P}(k-1)\cdot\boldsymbol{\varphi}(k)}\right] \tag{3.62}$$

Modifications of the RLS methods differ for different values of λ.

A) Decreasing gain: if $\lambda_1 = \lambda_2 = 1$, the gain is decreasing and covariance matrix increases. This method can be used for stationary systems.

B) Constant exponential forgetting is for $\lambda_1 < 1$ and $\lambda_2 = 1$. The values of forgetting factor λ_1 are from the range <0.95; 0.99>. Parameter λ_1 influences gradual forgetting of the old values and the most weight is put on the last values. This relation can be described by criterion

$$J=\sum_{i=1}^{k}\lambda^{k-i}\varepsilon_i^2 \tag{3.63}$$

This algorithm can be used for systems with changing parameters.

C) Increasing exponential forgetting has forgetting parameters $\lambda_2 = 1$ and λ_1 is computed from

$$\lambda_1(k)=\lambda_0\lambda_1(k-1)+1-\lambda_0 \tag{3.64}$$

Typical values of the forgetting parameters are $\lambda_1(0)=\lambda_0\in\langle 0.95,0.99\rangle$. The value of this forgetting factor is asymptotically approaching to 1, which means that the old data is forgotten. This can be used for stationary systems because it prevents gain from very quick decreasing at the beginning of identification and results in quick convergence for estimations which are far from the optimal ones.

D) Changing exponential forgetting has again the value of forgetting parameter $\lambda_2 = 1$ and exponential forgetting λ_1 is recomputed in every step as

$$\lambda_1(k)=1-K\cdot\gamma(k)\cdot\varepsilon^2(k) \tag{3.65}$$

where K is a very small value (e.g. 0.001).

E) Directional forgetting. Modifications of the RLS method with exponential forgetting described above have one big disadvantage. If the time interval between the old and new information is very high, it can happen that covariance matrix **P** becomes semidefinite and the algorithm collapses. Estimation with directional forgetting [32] was made especially to stabilize of this problem. This algorithm forgets information only in the direction from which it comes. General description of this method can be formulated by the following equations:

$$r(k-1) = \boldsymbol{\varphi}^T(k) \cdot \mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k) \tag{3.66}$$

$$\boldsymbol{L}(k) = \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k)}{1 + r(k-1)} \tag{3.67}$$

$$\beta(k-1) = \begin{cases} \lambda_1(k-1) - \dfrac{1-\lambda_1(k-1)}{r(k-1)} & \text{pro } r(k-1) > 0 \\ 1 & \text{pro } r(k-1) = 0 \end{cases} \tag{3.68}$$

$$\mathbf{P}(k) = \mathbf{P}(k-1) - \frac{\mathbf{P}(k-1) \cdot \boldsymbol{\varphi}(k) \cdot \boldsymbol{\varphi}^T(k) \cdot \mathbf{P}(k-1)}{\beta^{-1}(k-1) + r(k-1)} \tag{3.69}$$

where λ_1 can be chosen similarly as in exponential forgetting.

F) Recursive identification with directional forgetting was modified in [33] to the *RLS adaptive directional forgetting*.

The description of this RLS method is similar to the previous case. The value of adaptive directional forgetting λ_1 is calculated for each sampling period according to relation

$$\lambda_1(k-1) = \left\{ 1 + (1+\rho_i)\left[\ln\left(1 + r(k-1)\right)\right] + \left[\frac{(\upsilon(k-1)+1)\eta(k-1)}{1 + r(k-1) + \eta(k-1)} - 1 \right] \frac{r(k-1)}{1 + r(k-1)} \right\}^{-1} \tag{3.70}$$

where

$$\eta(k)=\frac{\hat{e}^2(k)}{\kappa(k)};\quad \upsilon(k)=\lambda_1(k)\left[(\upsilon(k-1)+1\right];\quad \kappa(k)=\lambda_1(k)\left[\kappa(k-1)+\frac{\hat{e}^2(k-1)}{1+r(k-1)}\right] \tag{3.71}$$

are auxiliary variables. The starting values for this method can be $\lambda_1(0)=1$, $\kappa(0)=0.001$, $\upsilon(0)=10^{-6}$, $\rho_i=0.99$.

The choice of the apriory information for the identification has in some cases a big importance for adaptive control results because the initial estimate of the parameters must represent real behaviour of the system. A bad first shot can result in wrong incialization of the controller and non-optimal responses.

POLYNOMIAL CONTROL SYSTEM SYNTHESIS

The polynomial synthesis [37] and [38] is one of the methods used in adaptive control for control synthesis of the system. This method is based on the input-output model of the controlled system or its transfer function. It can be classified as an algebraic method and is based on algebraic operations in the ring of polynomials. Polynomials are usually described in *s*-plane for continuous systems, in *z*-plane for discrete systems and in δ-plane for systems which come from δ-models of both the controlled system and the controller too ([55] and [56]).

One of the biggest advantages of the polynomial method compared to the conventional method is that it provides not only relations for computing of the controller's parameters but the structure of the controller too. This structure fulfils general requirements for control systems and input signals (reference signal and disturbance) and it can be used for controlling of the systems with negative properties from the control point of view, such as non-minimum phase systems or unstable systems. Another advantage is that the resulted relations are easily programmable.

Polynomials in the numerator and denominator of the transfer function of the controller result from the solution of Diophantine equations, which have so called *characteristic polynomial of the closed loop system* on the right side of the equation. The roots of this polynomial are then poles of the closed-loop system, which affects the quality of control. The method of choosing the poles is called *Pole-placement* or *Pole-assignment* [38].

The polynomial method can be used not only for the configuration with the feedback controller (1DOF configuration) but for configurations with the feedforward controller too (2DOF, 2½DOF etc.) [40].

Basic Control Requirements

The basic control requirements are defined in the following items:

A) Bounded Input-Bounded Output (BIBO) stability means that a system is BIBO stable if the bounded input results in a bounded output response [14]. This definition is not very suitable for closed-loop control systems where we examine not the only outer stability but also inner stability. It means that not only input and output signals must be bounded but signals inside the systems must be bounded too for BIBO stability of the closed-loop control system [57].

B) Inner properness of the control system is fulfilled if all elements are proper, i.e. degrees of denominators of transfer functions are equal or grater than numerators. The system with transfer function

$$G(s)=\frac{b(s)}{a(s)} \tag{3.72}$$

is:

proper if $\deg a(s) \geq \deg b(s)$

strictly proper if $\deg a(s) > \deg b(s)$

non-strictly proper if $\deg a(s) = \deg b(s)$

C) Asymptotic tracking of the reference signal means that the control error approaches to zero for infinite time. The output variable then asymptotically tracks reference signal (wanted value), i.e.

$$\lim_{t\to\infty} e(t) = 0 \tag{3.73}$$

D) Disturbance attenuation is the last control requirement. There are usually several disturbances which affect the control system and our goal is to suppress these negative influences to fulfil condition (3.73).

1DOF Control System Configuration

As already written, there are several types of control system configurations. The first one is configuration with *one degree-of-freedom* (1DOF) displayed on Figure 3.2. This combination has a controller only in the feedback part and control disturbance $e(t)$ is assigned as an input variable to this controller.

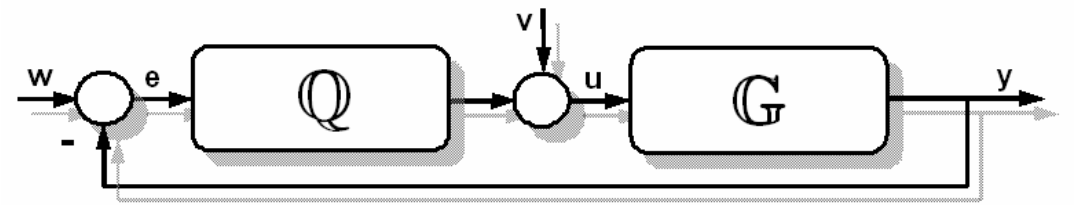


Figure 3.2 One degree-of-freedom (1DOF) control system configuration

Block Q in Figure 3.2 represents the transfer function of the controller, G denotes the transfer function of the plant, w is the reference signal, e is used for the control error, v is the disturbance at the input to the system, u determines the input variable, and finally y is the output variable.

The transfer function of the controlled system in complex s-plane can be described similar by to Equation (3.72). Polynomials $a(s)$ and $b(s)$ are commensurable polynomials

in complex s-plane. The realizability condition is fulfilled if the system is proper, i.e. $\deg a(s) \geq \deg b(s)$.

The transfer function of the controller then is

$$Q(s) = \frac{q(s)}{p(s)} \tag{3.74}$$

where polynomials $p(s)$ and $q(s)$ are again commensurable polynomials, and the condition of properness in this case is $\deg p(s) \geq \deg q(s)$.

Transfer functions of the reference signal $W(s)$ and disturbance $V(s)$ are

$$W(s) = \frac{h_w(s)}{f_w(s)} \text{ and } V(s) = \frac{h_v(s)}{f_v(s)} \tag{3.75}$$

where the degrees of polynomials in denominators and numerators are again based on the condition of properness: $\deg f_w(s) \geq \deg h_w(s)$ and $\deg f_v(s) \geq \deg h_v(s)$.

The reference signal $W(s)$ and disturbances $V(s)$ are chosen from the range of step functions, which means that polynomials in denominators are $f_w = f_v = s$.

The relation for the Laplace transform of the output variable $Y(s)$ can be obtained from the transfer function of the system $G(s)$:

$$G(s) = \frac{Y(s)}{U(s)} \Rightarrow Y(s) = G(s) \cdot U(s) \tag{3.76}$$

where $U(s)$ from Figure 3.2 is

$$U(s) = Q(s) \cdot E(s) + V(s) = Q(s) \cdot \left[W(s) - Y(s) \right] + V(s) \tag{3.77}$$

This relation together with polynomials $a(s)$, $b(s)$, $p(s)$ and $q(s)$ instead of Laplace transforms $G(s)$ and $Q(s)$ inserted into Equation (3.76) results in

$$Y(s)=\frac{b(s)q(s)}{a(s)p(s)+b(s)q(s)}\cdot W(s)+\frac{a(s)p(s)}{a(s)p(s)+b(s)q(s)}\cdot V(s) \tag{3.78}$$

Denominators for both parts have the same form. This polynomial is called characteristic polynomial of the closed loop and it can be assigned in one polynomial

$$a(s)p(s)+b(s)q(s)=d(s) \tag{3.79}$$

The stability of the system is fulfilled by the feedback part of the controller with transfer function $Q(s)$ [38], where polynomials $p(s)$ and $q(s)$ are computed from Diophantine equation (3.79). The stability of the system is obtained for a stable polynomial $d(s)$ on the right side.

Asymptotic tracking of the reference signal is attained if polynomial $p(s)$ in the denominator of Equation (3.74) includes least common divisor of polynomials $f_w(s)$ and $f_v(s)$. This can be obtained for polynomial $p(s)$ rewritten to form

$$p(s)=f(s)\cdot\tilde{p}(s) \tag{3.80}$$

where $f(s)$ is the least common divisor mentioned above. This polynomial is $f(s)=f_w(s)=f_v(s)=s$ for signals from the range of step functions.

Diophantine equation (3.79) is then

$$a(s)f(s)\tilde{p}(s)+b(s)q(s)=d(s) \tag{3.81}$$

and the transfer function of the controller is

$$\tilde{Q}(s)=\frac{q(s)}{f(s)\cdot\tilde{p}(s)} \tag{3.82}$$

Polynomials $a(s)$ and $b(s)$ in Diophantine equation (3.81) are known from identification. Our task is to find coefficients of polynomials $q(s)$ and $\tilde{p}(s)$. The method

of uncertain coefficients which compares coefficients of individual *s*-powers can be used for computing of parameters of polynomials $\tilde{p}(s)$ and $q(s)$.

Inner properness conditions must be fulfilled, i.e. $\deg a(s) \geq \deg b(s)$ and $\deg p(s) \geq \deg q(s)$ and because

$$\deg\left(a(s)\cdot f(s)\cdot \tilde{p}(s)\right) \geq \deg\left(b(s)\cdot q(s)\right) \tag{3.83}$$

the degree of polynomial $d(s)$ is then

$$\deg d(s) = \deg\left(a(s) f(s) \tilde{p}(s)\right) = \deg a(s) + \deg f(s) + \deg \tilde{p}(s) \tag{3.84}$$

The number of unknown parameters in (3.81) is

$$\deg \tilde{p}(s) + \deg q(s) + 2 \tag{3.85}$$

and the number of equations is then

$$\deg d(s) + 1 = \deg a(s) + \deg f(s) + \deg \tilde{p}(s) + 1 \tag{3.86}$$

The number of unknown parameters must be equal to the number of equations and therefore

$$\begin{aligned} &\deg a(s) + \deg f(s) + \deg \tilde{p}(s) + 1 = \deg \tilde{p}(s) + \deg q(s) + 2 \Rightarrow \\ &\quad \Rightarrow \deg q(s) = \deg a(s) + \deg f(s) - 1 \end{aligned} \tag{3.87}$$

The properness condition is $\deg p(s) \geq \deg q(s)$, it means that

$$\begin{aligned} &\deg p(s) = \deg f(s)\tilde{p}(s) = \deg f(s) + \deg \tilde{p}(s) \geq \deg q(s) \\ &\quad \deg f(s) + \deg \tilde{p}(s) \geq \deg a(s) + \deg f(s) - 1 \Rightarrow \\ &\qquad \Rightarrow \deg \tilde{p}(s) \geq \deg a(s) - 1 \end{aligned} \tag{3.88}$$

2DOF Control System Configuration

The configuration with *two degrees-of-freedom* (2DOF) has a controller divided into two main parts – the feedback segment with the transfer function $Q(s)$, which has output variable $y(t)$ on the input and the feedforward segment with transfer function $R(s)$ – see Figure 3.3.

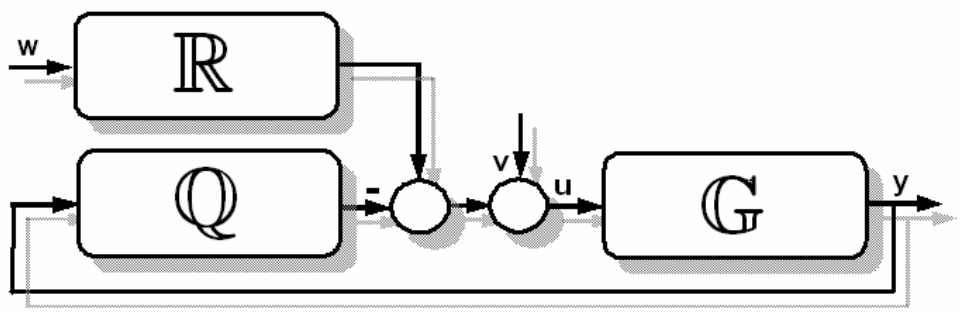


Figure 3.3 Two degrees-of-freedom (2DOF) control system configuration

This part has reference signal $w(t)$ on the input. We can say that this controller has two inputs (output variable $y(t)$ and reference signal $w(t)$) and one output from the controller, $u(t)$.

Transfer functions of both parts are

$$Q(s)=\frac{q(s)}{p(s)},\ R(s)=\frac{r(s)}{p(s)} \tag{3.89}$$

where polynomials $p(s)$, $q(s)$ and $r(s)$ are complex s-plane, and properness conditions are $\deg p(s)\geq \deg q(s)$ and $\deg p(s)\geq \deg r(s)$.

Laplace transform of the input variable $U(s)$ is computed from Figure 3.3.

$$U(s)=R(s)W(s)-Q(s)Y(s)+V(s) \tag{3.90}$$

and if we input it similar by as in the previous case in (3.76), with some simplifications the relation is

$$Y(s)=\frac{b(s)r(s)}{a(s)p(s)+b(s)q(s)}\cdot W(s)+\frac{b(s)p(s)}{a(s)p(s)+b(s)q(s)}\cdot V(s) \tag{3.91}$$

Both denominators are again the characteristic polynomial $d(s)=a(s)p(s)+b(s)q(s)$.

Stability is again fulfilled by polynomials $q(s)$ and $p(s)$ of the feedback part of the controller the parameters of which are computed from Diophantine equation (3.79). Asymptotic tracking is obtained by the solution of the second Diophantine equation

$$t(s)f_w(s)+b(s)r(s)=d(s) \tag{3.92}$$

where $t(s)$ is only an additional polynomial which is used only for the solution of Equation (3.92) and not in transfer functions.

On the other hand, disturbance attenuation is gained in the case that polynomial $p(s)$ in the denominator of the $Q(s)$ and $R(s)$ is divisible by polynomial $f_v(s)$. We can then rewrite this polynomial to the form of

$$p(s)=f_v(s)\cdot\tilde{p}(s) \tag{3.93}$$

Diophantine equation (3.79) is then

$$a(s)f_v(s)\tilde{p}(s)+b(s)q(s)=d(s) \tag{3.94}$$

and transfer functions of feedback and feedforward segments are

$$\tilde{Q}(s)=\frac{q(s)}{f_v(s)\cdot\tilde{p}(s)},\ \tilde{R}(s)=\frac{r(s)}{f_v(s)\cdot\tilde{p}(s)} \tag{3.95}$$

The degree of characteristic polynomial $d(s)$ is computed from (3.94) as

$$\deg d(s)=\deg\left(a(s)f_v(s)\tilde{p}(s)\right)=\deg a(s)+\deg f_v(s)+\deg\tilde{p}(s) \tag{3.96}$$

The number of unknown parameters is similar to the previous case

$$\deg \tilde{p}(s) + \deg q(s) + 2 \tag{3.97}$$

and the number of equations is

$$\deg a(s) + \deg f_v(s) + \deg \tilde{p}(s) + 1 \tag{3.98}$$

The relation for the degree of polynomial $q(s)$ is computed from the condition that the number of unknown parameters must be equal to the number of equations, i.e.

$$\begin{aligned} &\deg \tilde{p}(s) + \deg q(s) + 2 = \deg a(s) + \deg f_v(s) + \deg \tilde{p}(s) + 1 \Rightarrow \\ &\qquad \Rightarrow \deg q(s) = \deg a(s) + \deg f_v(s) - 1 \end{aligned} \tag{3.99}$$

The degree of polynomial $\tilde{p}(s)$ is computed via

$$\deg \tilde{p}(s) = \deg a(s) - 1 + k_d \tag{3.100}$$

with constant k_d on the right side and and the degree of the polynomial $d(s)$ in Equation (3.96) is then

$$\deg d(s) = 2\deg a(s) + \deg f_v(s) - 1 + k_d \tag{3.101}$$

The degree of polynomial $d(s)$ from the second Diophantine equation (3.92) is

$$\deg d(s) = \deg t(s) + \deg f_w(s) \tag{3.102}$$

and the degree of polynomial $r(s)$ is obtained from the comparison of the number of unknown parameters and number of equations:

$$\begin{aligned} &\deg t(s) + \deg f_w(s) + 1 = \deg t(s) + \deg r(s) + 2 \Rightarrow \\ &\qquad \Rightarrow \deg r(s) = \deg f_w(s) - 1 \end{aligned} \tag{3.103}$$

Finally, the degree of auxiliary polynomial $t(s)$ can be computed as

$$\deg t(s) = 2\deg a(s) + \deg f_v(s) - 1 - \deg f_w(s) + k_d \tag{3.104}$$

It is clear that the degree cannot be negative, therefore we choose constant k_d so that deg $t(s)$ is at least zero. The value of this constant can be obtained from the condition of properness $\deg p(s) \geq \deg r(s)$:

$$\begin{aligned} &\deg f_w(s) - 1 \geq \deg a(s) - 1 + \deg f_v(s) + k_d \Rightarrow \\ &\Rightarrow k_d \geq \deg f_w(s) - \deg a(s) - \deg f_v(s) \end{aligned} \tag{3.105}$$

and if $k_d < 0$, then $k_d = 0$.

Pole-assignment Method

Several methods are used for designing polynomial $d(s)$ based on the *Pole-placement* or *Pole-assignment method*. It is usually connected with the polynomial synthesis and fulfils control requirements [37].

The control system is stable if polynomial $d(s)$ on the right side of Diophantine equations (3.81) and (3.92) is stable. This condition is accomplished if the root of the polynomial lies in on the left side of the complex plane – see Figure 3.4.

Polynomial $d(s)$ can generally described as

$$d(s) = \prod_{i=1}^{\deg d(s)} (s + s_i) \tag{3.106}$$

where $s_i = \alpha_i + \omega_i j$ are *roots* of the polynomial. The stability condition described in the previous paragraph means that α_i must be less zero. There are a lot of ways and rules how to choose these roots. *Complex conjugate pairs of roots* results in periodic course of the output variable. On the other hand, the output variable has aperiodic course for $\omega_i = 0$.

We can generally say that selection of real (*Re*) and imaginary (*Im*) parts affects overshoots and settling time of the output variable.

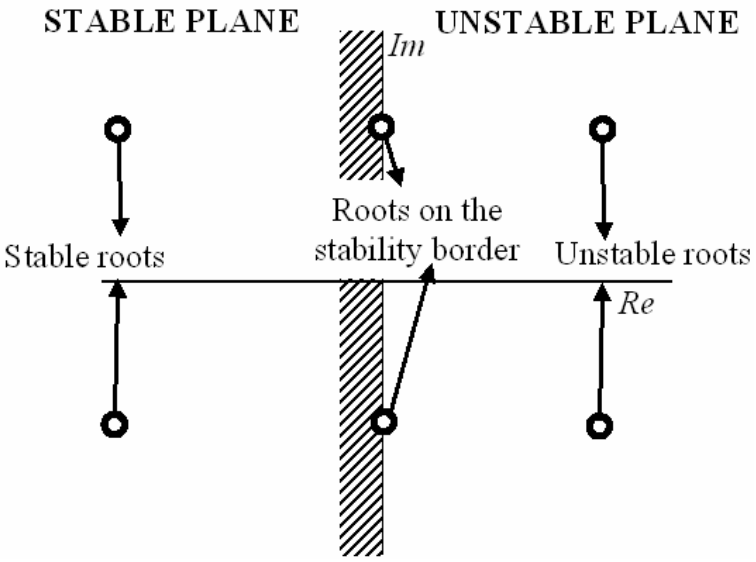


Figure 3.4 Stability in complex plane

The simplest way how to choose roots of polynomial $d(s)$ is selection of double, triple etc. multiple roots:

$$d(s)=(s+\alpha)^m ; d(s)=(s+\alpha_1)^{m/2}\cdot(s+\alpha_2)^{m/2},\ldots \tag{3.107}$$

For example, if polynomial $d(s)$ is of the fourth degree, we can select two aperiodic double roots, i.e.

$$d(s)=(s+\alpha_1)^2\cdot(s+\alpha_2)^2 \tag{3.108}$$

We can obtain similar roots for the sixth degree of $d(s)$ etc.

However, this method has one disadvantage, there is no rule how to choose roots α. One way how to overcome this problem is to connect choosing of polynomial $d(s)$ with parameters of the controlled system. This can be done through *spectral factorization* [39]. A big advantage of this method is that it can make stable roots from every polynomial, even if it is unstable.

Polynomial $d(s)$ can be divided into two parts – $m(s)$ and $n(s)$, so

$$d(s) = m(s) \cdot n(s) \tag{3.109}$$

where polynomial $n(s)$ is computed from the spectral factorization of polynomial $a(s)$ in the denominator of the transfer function $G(s)$ (3.72)

$$n^*(s) \cdot n(s) = a^*(s) \cdot a(s) \tag{3.110}$$

and polynomial $m(s)$ is a stable one

$$m(s) = (s + \alpha_i)^{\deg d - \deg n} \tag{3.111}$$

where $\alpha_i > 0$ are $(\deg d - \deg n)$ optional stable roots, usually called poles of the control system. A disadvantage of this method is that it still has an uncertainty in polynomial $m(s)$.

The third method used in this work combines spectral factorization and theory of the *Linear Quadratic (LQ) tracking*. The LQ approach is based on an optimal control theory and in addition to the basic control requirements, it minimize the cost function in the complex domain

$$J_{LQ} = \int_0^\infty \{\mu_{LQ} \cdot e^2(t) + \varphi_{LQ} \cdot \dot{u}^2(t)\} dt \tag{3.112}$$

where $\varphi_{LQ} > 0$ and $\mu_{LQ} \geq 0$ are weighting coefficients, $e(t)$ is control error and $\dot{u}(t)$ denotes difference of the input variable. Polynomial $d(s)$ in this case is

$$d(s) = g(s) \cdot n(s) \tag{3.113}$$

Polynomials $n(s)$ and $g(s)$ are computed from spectral factorization

$$\begin{aligned}\left(a\cdot f\right)^{*}\cdot\varphi_{LQ}\cdot a\cdot f+b^{*}\cdot\mu_{LQ}\cdot b&=g^{*}\cdot g\\ n^{*}\cdot n&=a^{*}\cdot a\end{aligned}\tag{3.114}$$

and for control variable $u(t)$ and disturbance $v(t)$ from the ring of step functions $f(s) = s$. The resulted controller is strictly proper and the degree of polynomial $d(s)$ is computed via

$$\deg d=\deg\left(g\cdot n\right)=2\deg a+1\tag{3.115}$$

3.2.2 Predictive Control

The main idea of predictive control is to calculate the control sequence from the actual time point minimizing the deviation of the reference signal and the output signal of the plant in the future horizon. The future values of the reference signal are given in advance or are assumed to be equal to the present one. The future values of the plant can be predicted from a process model. If disturbances are measurable, then their future values are predicted using some assumptions.

The basic structure of the predictive control can be seen in Figure 3.5 [58].

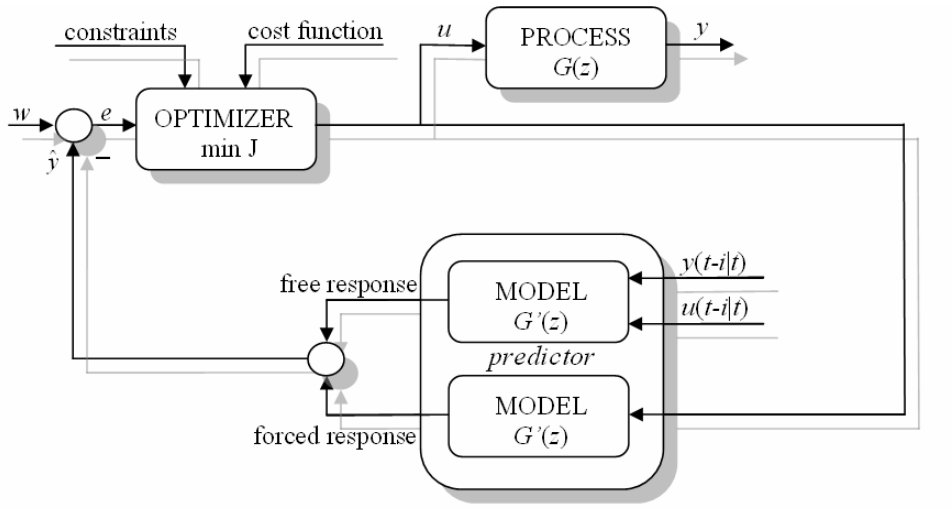


Figure 3.5 Basic structure of the predictive control system

The total predicted response of the system, $\hat{y}$, consists of two parts. The first part, *free response*, is the predicted behaviour of the output $y(t+j|t)$ based on old values of outputs $y(t-i|t)$ and inputs $u(t-i|t)$. The second part is called *forced response* and represents the output computed from the optimization criterion.

The sum of both components results in total prediction $y(t+j|t)$ for linear systems. The future error is then obtained by subtracting of this output from future reference signal $w(t+j|t)$, i.e.

$$e(t+j|t) = w(t+j|t) - y(t+j|t), \text{ for } j = 1,\ldots N \tag{3.116}$$

The action value (input variable) is then calculated to force the output variable to the wanted value (reference signal).

Generalized Predictive Control (GPC) is one of the most popular predictive methods based on Model Predictive Control (MPC) [44], and has been successfully used in praxis for different types of control problems from this time.

The GPC has many common ideas with the ordinary predictive methods but it has some differences to such as the solution of the GPC controller is analytical, it can be used for unstable and non-minimum phase systems etc.

FORMULATION OF GENERALIZED PREDICTIVE CONTROL

The general single-input single-output (SISO) after linearization can be described through the discrete backshift operators z^{-1} as

$$A(z^{-1}) \cdot y(t) = z^{-d} \cdot B(z^{-1}) \cdot u(t-1) + C(z^{-1}) \cdot e(t) \tag{3.117}$$

where $u(t)$ is control variable, $y(t)$ output variable, $e(t)$ denotes a zero mean white noise, and d is dead time of the system. Polynomials $A(z^{-1})$, $B(z^{-1})$ and $C(z^{-1})$ are

$$A\left(z^{-1}\right)=1+a_1z^{-1}+a_2z^{-2}+\ldots+a_{n_a}z^{-n_a}$$
$$B\left(z^{-1}\right)=b_0+b_1z^{-1}+b_2z^{-2}+\ldots+b_{n_b}z^{-n_b} \tag{3.118}$$
$$C\left(z^{-1}\right)=1+c_1z^{-1}+c_2z^{-2}+\ldots+c_{n_c}z^{-n_c}$$

Equation (3.117) is called the *Controller Auto-Regressive Moving-Average* (CARMA) *model*. This model is not suitable in most industrial processes where disturbances are non-stationary. In these cases, the integrated CARMA (CARIMA) model is more suitable

$$A\left(z^{-1}\right)\cdot y\left(t\right)=z^{-d}\cdot B\left(z^{-1}\right)\cdot u\left(t-1\right)+C\left(z^{-1}\right)\cdot\frac{e\left(t\right)}{\Delta} \tag{3.119}$$

where $\Delta=1-z^{-1}$.

The GPC algorithm can be then formulated as minimization of the cost function

$$J_{GPC}=\sum_{j=N_1}^{N_2}\delta_u\left(j\right)\left[\hat{y}\left(t+j\middle|t\right)-w\left(t+j\right)\right]^2+\sum_{j=1}^{N_u}\lambda_u\left(j\right)\left[\Delta u\left(t+j-1\right)\right]^2 \tag{3.120}$$

where $\hat{y}\left(t+j\middle|t\right)$ is an optimum j-ahead prediction of the output on data up to time t, further, N_1 and N_2 denote minimum and maximum costing horizons, respectively, N_u is control horizon, $w\left(t+j\right)$ means reference signal, Δu stands for manipulated variable and finally $\delta_u(j)$ and $\lambda_u(j)$ denote weighting sequences. The values of these factors are for simplification assigned as $\delta_u = 1$, and λ_u is constant through the whole time interval of the control.

COMPUTATION OF GENERALIZED PREDICTIVE CONTROL

The object of predictive control can be formulated as collection of the future values of the input variables $u(t)$, $u(t+1)$, … which drive the future values of controlled variable $y(t+j)$ to reference signal $w(t+j)$ by minimizing of the cost function J_{GPC}.

If we multiply all parts of Equation (3.119) by element $\Delta E_j\left(z^{-1}\right)\cdot z^j$, this equation has form

$$A\left(z^{-1}\right)\cdot\Delta\cdot E_j\left(z^{-1}\right)\cdot y\left(t+j\right)=B\left(z^{-1}\right)\cdot\Delta\cdot E_j\left(z^{-1}\right)\cdot u\left(t+j-d-1\right)+E_j\left(z^{-1}\right)\cdot e\left(t+j\right) \quad (3.121)$$

Now we must introduce a new Diophantine equation because of the solubility of Equation (3.121):

$$1=\Delta\cdot E_j\left(z^{-1}\right)\cdot A\left(z^{-1}\right)+z^{-j}F_j\left(z^{-1}\right) \quad (3.122)$$

Equation (3.121) is then

$$\left[1-z^{-j}F_j\left(z^{-1}\right)\right]y\left(t+j\right)=E_j\left(z^{-1}\right)B\left(z^{-1}\right)\Delta u\left(t+j-d-1\right)+E_j\left(z^{-1}\right)e\left(t+j\right) \quad (3.123)$$

which can be formally rewritten to the form

$$\hat{y}\left(t+j|t\right)=G_j\left(z^{-1}\right)\Delta u\left(t+j-d-1\right)+F_j\left(z^{-1}\right)y\left(t\right) \quad (3.124)$$

where $G_j\left(z^{-1}\right)=E_j\left(z^{-1}\right)B\left(z^{-1}\right)$, degrees of E_j and F_j are $\deg E_j=j-1$ and $\deg F_j=n_a$, respectively. These polynomials can be obtained through the dividing 1 by $\Delta A\left(z^{-1}\right)$ until the remaining part can be factorized as $z^{-j}F_j\left(z^{-1}\right)$, and we can define them as

$$\begin{aligned}F_j\left(z^{-1}\right)&=f_{j,0}+f_{j,1}z^{-1}+\ldots+f_{j,na}z^{-na}\\E_j\left(z^{-1}\right)&=e_{j,0}+e_{j,1}z^{-1}+\ldots+e_{j,j-1}z^{-j-1}\end{aligned} \quad (3.125)$$

If the same technique is used for deriving of the polynomials E_{j+1} and F_{j+1}, i.e. 1 is divided by $\Delta A\left(z^{-1}\right)$ until the remaining part can be factorized as $z^{-(j+1)}F_{j+1}\left(z^{-1}\right)$; then polynomials F_{j+1} and E_{j+1} are

$$\begin{aligned} F_{j+1}\left(z^{-1}\right) &= f_{j+1,0} + f_{j+1,1}z^{-1} + \ldots + f_{j+1,na}z^{-na} \\ E_{j+1}\left(z^{-1}\right) &= e_{j+1,0} + e_{j+1,1}z^{-1} + \ldots + e_{j+1,j-1}z^{-(j-1)} \end{aligned} \tag{3.126}$$

It is clear that the polynomial E_j (or F_j) from the previous step can be used for the derivation of polynomial E_{j+1}(F_{j+1}):

$$E_{j+1}\left(z^{-1}\right) = E_j\left(z^{-1}\right) + e_{j+1,j}z^{-j} \tag{3.127}$$

where $e_{j+1,j} = f_{j,0}$.

Polynomial G_{j+1} can be computed recursively again from equation

$$G_{j+1}\left(z^{-1}\right) = E_{j+1}\left(z^{-1}\right)\cdot B\left(z^{-1}\right) = \left[E_j\left(z^{-1}\right) + f_{j,0}z^{-j}\right]B\left(z^{-1}\right) \tag{3.128}$$

which means that G_{j+1} come from the G_j:

$$G_{j+1}\left(z^{-1}\right) = G_j\left(z^{-1}\right) + f_{j,0}z^{-j}B\left(z^{-1}\right) \tag{3.129}$$

The first coefficient of polynomial G_{j+1} is identical with the first coefficient in G_j and the remaining coefficients are computed from equation

$$g_{j+1,j+i} = g_{j,j+i} + f_{j,0}b_i, \text{ for } i = 0, 1, \ldots, n_b \tag{3.130}$$

Equation (3.117) takes into account the dead time of the system, d, and we must include this time into the prediction horizon, i.e. $N_1 = d + 1$, $N_2 = d + N$ and $N_u = N$.

Now we can formulate equations for future predicted output values:

$$\begin{aligned}
\hat{y}\left(t+d+1\middle|t\right) &= G_{d+1}\Delta u\left(t\right)+F_{d+1}y\left(t\right)\\
\hat{y}\left(t+d+2\middle|t\right) &= G_{d+2}\Delta u\left(t+1\right)+F_{d+2}y\left(t\right)\\
&\vdots\\
\hat{y}\left(t+d+N\middle|t\right) &= G_{d+N}\Delta u\left(t+N-1\right)+F_{d+N}y\left(t\right)
\end{aligned} \tag{3.131}$$

which is in the vector form

$$\boldsymbol{y}=\boldsymbol{G}\boldsymbol{u}+\boldsymbol{F}\left(z^{-1}\right)y\left(t\right)+\boldsymbol{G'}\left(z^{-1}\right)\Delta u\left(t-1\right) \tag{3.132}$$

where vectors $\boldsymbol{y}$, $\boldsymbol{u}$, $\boldsymbol{G}$, $\boldsymbol{G'}(z^{-1})$ and $\boldsymbol{F}(z^{-1})$ are

$$\boldsymbol{y}=\begin{bmatrix}\hat{y}\left(t+d+1\middle|t\right)\\ \hat{y}\left(t+d+2\middle|t\right)\\ \vdots\\ \hat{y}\left(t+d+N\middle|t\right)\end{bmatrix} \qquad \boldsymbol{u}=\begin{bmatrix}\Delta u\left(t\right)\\ \Delta u\left(t+1\right)\\ \vdots\\ \Delta u\left(t+N-1\right)\end{bmatrix}$$

$$\boldsymbol{G}=\begin{bmatrix}g_0 & 0 & \dots & 0\\ g_1 & g_0 & \dots & 0\\ \vdots & & \ddots & \\ g_{N-1} & g_{N-2} & \dots & g_0\end{bmatrix} \qquad \boldsymbol{G'}\left(z^{-1}\right)=\begin{bmatrix}\left[G_{d+1}\left(z^{-1}\right)-g_0\right]z\\ \left[G_{d+2}\left(z^{-1}\right)-g_0-g_1z^{-1}\right]z^2\\ \vdots\\ \left[G_{d+N}\left(z^{-1}\right)-g_0-g_1z^{-1}-\dots-g_{N-1}z^{-(N-1)}\right]z^N\end{bmatrix}$$

$$\boldsymbol{F}\left(z^{-1}\right)=\begin{bmatrix}F_{d+1}\left(z^{-1}\right)\\ F_{d+2}\left(z^{-1}\right)\\ \vdots\\ F_{d+N}\left(z^{-1}\right)\end{bmatrix}$$

The last two parts of Equation (3.132) depend only on the past values and we can group them into one variable, **f**:

$$\boldsymbol{y} = \boldsymbol{G} \cdot \boldsymbol{u} + \mathbf{f} \tag{3.133}$$

The cost function (3.120) can be now rewritten to the vector form

$$J = \left(\boldsymbol{G} \cdot \boldsymbol{u} + \mathbf{f} - \boldsymbol{w}\right)^T \left(\boldsymbol{G} \cdot \boldsymbol{u} + \mathbf{f} - \boldsymbol{w}\right) + \lambda_u \cdot \boldsymbol{u}^T \cdot \boldsymbol{u} \tag{3.134}$$

Where the vector of reference values is

$$\boldsymbol{w} = \left[w\left(t + d + 1\right), w\left(t + d + 2\right), \ldots, w\left(t + d + N\right) \right]^T \tag{3.135}$$

and (3.134) can be rewritten to

$$J_{GPC} = \frac{1}{2} \boldsymbol{u}^T \boldsymbol{H} \boldsymbol{u} + \boldsymbol{b}^T \boldsymbol{u} + \mathbf{f}_0 \tag{3.136}$$

where

$$\begin{aligned} \boldsymbol{H} &= 2\left(\boldsymbol{G}^T \boldsymbol{G} + \lambda_u \boldsymbol{I}\right) \\ \boldsymbol{b}^T &= 2\left(\mathbf{f} - \boldsymbol{w}\right)^T \boldsymbol{G} \\ \mathbf{f}_0 &= \left(\mathbf{f} - \boldsymbol{w}\right)^T \left(\mathbf{f} - \boldsymbol{w}\right) \end{aligned} \tag{3.137}$$

The goal of the predictive control is to minimize cost function J_{GPC} which means that we set $J_{GPC} = 0$ in (3.136) which leads to control law:

$$u = \left(\boldsymbol{G}^T \boldsymbol{G} + \lambda_u \boldsymbol{I}\right)^{-1} \boldsymbol{G}^T \left(\boldsymbol{w} - \mathbf{f}\right) \tag{3.138}$$

3.3 Main Types of Chemical Reactors

Chemical reactors are special devices used in chemical engineering for manufacturing different chemical products. There are two main types of chemical reactors – *tank reactors* and *tubular reactors* [4].

The main variables which are observed are the volume of the reactor, reactant's and product's concentrations, input, inside and output temperature, pressure, concentrations of the components, heat capacities, densities, heat transfer coefficients etc. Some of them are important and must be taken into account, but some of them must be neglected or set to constant because of the complexity of the mathematical description.

Tank reactors are usually stirred to ensure an efficient course of the reaction inside the vessel. These reactors are called stirred-tank reactors and can be divided from the feeding point of view into *batch*, *semi-batch* and *continuous* types. All stirred reactors can be mathematically described by a set of ODE.

A *batch reactor* (Figure 3.6) is the simplest type of stirred chemical reactors.

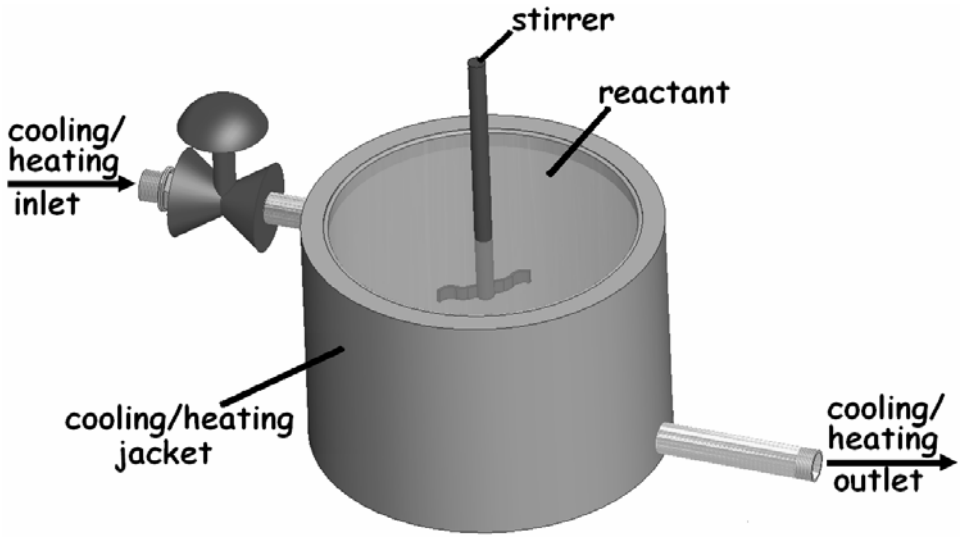


Figure 3.6 Batch reactor

It can be characterized by a vessel of a given volume, with all reactants added at the same time – at the beginning of the process. The concentration of the reactant

decreases continuously with time. At the end of the process the reactor is emptied, cleaned and another batch can be filled in the same reactor. This is very simple and provides great flexibility of the basic equipment. However, the downtime needed for loading and cleaning of the reactor are the disadvantages. Batch operations are often ideal for small scale flexible production, high cost and low output production.

On the other hand, for many reactions the pure batch operation is not suitable because of safety or selectivity reasons. In this case we can use a *semi-batch system* where one reactant is put at the reactor in the beginning and other components can be added to the reactor during the operation at different times (Figure 3.7). Semi-batch operation allows for changing of the reactant concentration in a very flexible way, and it is easier to control the operations. The flexibility of operation is generally similar to that of a batch reactor system.

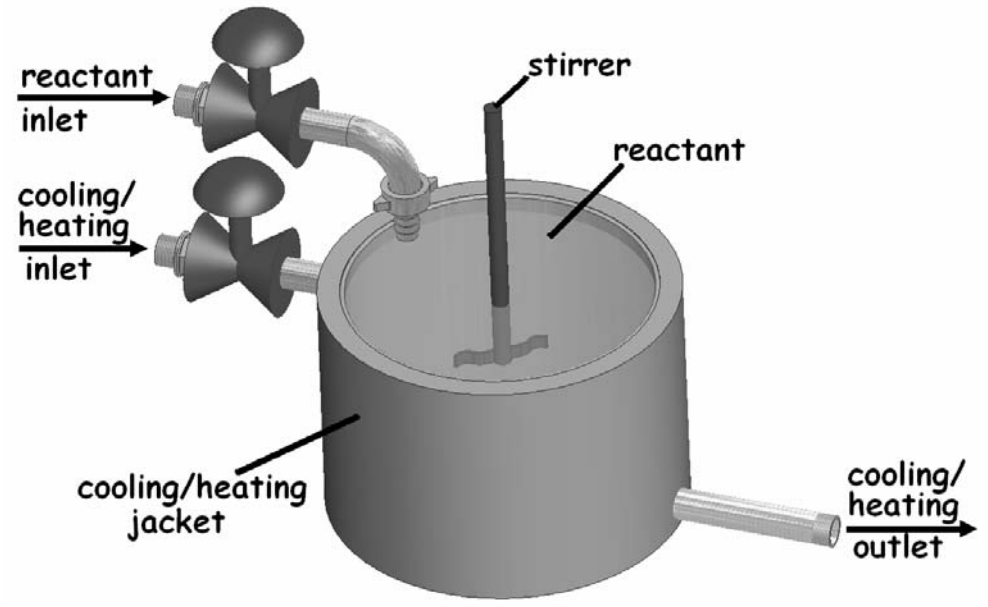


Figure 3.7 Semi-batch reactor

Continuous Stirred Tank Reactors, CSTRs, (Figure 3.8) are often used because of their good control properties. Feeding and unloading can be done continuously, which can be easily used for control where we want to affect product properties by the feeding speed,

for example. One of the disadvantages, however, is limited use for different types of reactions.

CSTRs are often connected parallelly or in series, which enables to utilize economic benefits of CSTR. The product from the first reactor is the input to the next one.

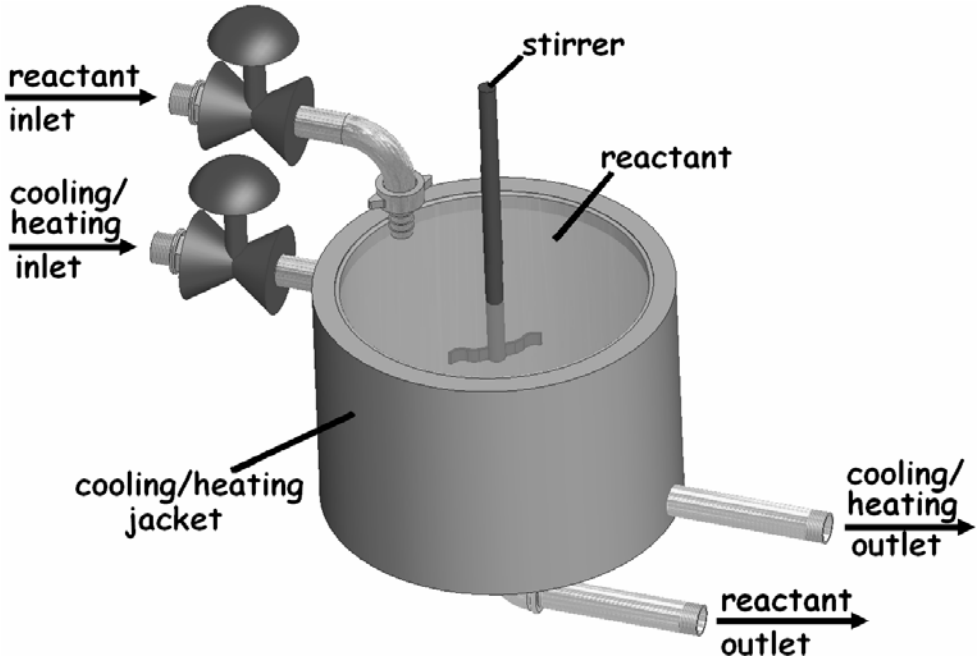


Figure 3.8 Continuous stirred tank reactor

An infinite number of CSTRs or infinitely small CSTRs operating in series create a *tubular chemical reactor*, which is another main type of chemical reactors. It is called in some literature *Plug-Flow Reactor* (PFR). In the tubular chemical reactor all reactants and products flow continuously along the length of the reactor – see Figure 3.9. It is usually considered with plug flow of the reactant or cooling through the reactor to lower complexity. The variables then depend not only on the time variable, but also on the dimensional variable, which results in a set of PDE.

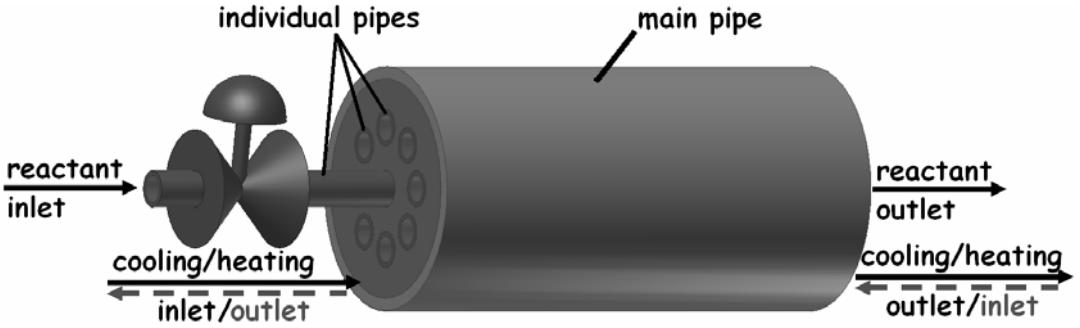


Figure 3.9 Tubular chemical reactor

As seen from previous figures, all types of reactors are displayed with the cooling/heating jacket. The use of the cooling and heating in the process depends on the type of reaction inside the reactor. The reaction which produces heat is called the *exothermic reaction* which needs cooling contrary to the *endothermic reaction* which needs heat in the jacket to start the reaction or to achieve better results.

The continuous stirred tank reactor belongs to the class of the *lumped-parameters systems*. The mathematical model of CSTR can be derived from the balances inside the reactor. The material balance can have general form:

$$q_r c_{iv} = q_r c_i - V_r \sum_{j=1}^{j_0} r_{ij} + V_r \frac{dc_i}{dt}, \quad \text{for } i = 1,...,i_0 \tag{3.139}$$

and general heat balances of the reactant and cooling/heating liquid are

$$q_r \rho_r c_{pr} T_{rv} + V_r \sum_{j=1}^{j_0} h_j r_j = q \rho_r c_{pr} T_r + A_r U (T_r - T_c) + V_r \rho_r c_p r \frac{dT_r}{dt} \tag{3.140}$$

$$q_c \rho_c c_{pc} T_{cv} + A_r U (T_r - T_c) = q_c \rho_c c_{pc} T_c + V_c \rho_c c_{pc} \frac{dT_c}{dt} \tag{3.141}$$

The symbols in the set (3.139) – (3.141) have following meaning: q are flow rates, c denotes concentrations, r is used for reaction speed, V states volume, t is time, ρ denotes density, c_p heat capacity, T is used for temperature, h means enthalpy, A_r is cooling/heating surface, U represents heat transfer coefficient. Indexes $(\cdot)_r$ and $(\cdot)_c$ relate to the reactant and

cooling/heating, respectively, $(\cdot)_v$ means input variable, $(\cdot)_i$ denotes i-th part of the component and $(\cdot)_j$ is used for number of reaction. The initial conditions for Equations (3.139) – (3.141) are obtained from the steady-state, i.e.

$$c_i(0) = c_i^s \text{ for } i = 1,\ldots, i_0;\ T_r(0) = T_r^s;\ T_c(0) = T_c^s \tag{3.142}$$

On the other hand, typical member of the *continuously distributed-parameters system* is tubular chemical reactor. The mathematical model of this system consists of the set of PDE which are obtained from the material and heat balances inside in this general form:

$$\begin{aligned}
&\frac{\partial c_i}{\partial t} + v_r \frac{\partial c_i}{\partial z} = \sum_{j=1}^{j_0} r_{ij}, \quad \text{for } i = 1,\ldots,i_0 \\
&\frac{\partial T_r}{\partial t} + v_r \frac{\partial T_r}{\partial z} = \frac{1}{\rho_r c_{pr}} \sum_{j=1}^{j_0} h_r r_j - \frac{4U_1}{d_1 \rho_r c_{pr}} (T_r - T_w) \\
&\frac{\partial T_w}{\partial t} = \frac{4}{(d_2^2 - d_1^2)\rho_w c_{pw}} \left[d_1 U_1 (T_r - T_w) + d_2 U_2 (T_c - T_w) \right] \\
&\frac{\partial T_c}{\partial t} \pm v_c \frac{\partial T_c}{\partial z} = \frac{4 m d_2 U_2}{(d_3^2 - m d_2^2)\rho_c c_{pc}} (T_w - T_c)
\end{aligned} \tag{3.143}$$

where ± in the last equation takes into the account co-current and counter-current cooling/heating in the jacket ("+" is used for co-current unlike "–" for counter-current cooling/heating).

The symbol c denotes concentrations, v are fluid velocities, r is used for reaction speed, t is time variable, z space variable, ρ denotes density, c_p heat capacity, T is used for temperature, h means enthalpy, A_r is cooling/heating surface, U represents heat transfer coefficient, d is diameter of the pipe and m means number of pipes. Indexes $(\cdot)_r$, $(\cdot)_w$ and $(\cdot)_c$ stands to the reactant, wall of the pipe or cooling/heating, respectively, $(\cdot)_v$ means input variable, $(\cdot)_i$ denotes i-th part of the component and $(\cdot)_j$ is used for number of reaction.

The initial conditions for the model (3.143) are:

$$c_i(z,0) = c_i^s(z), \quad T_r(z,0) = T_r^s(z), \quad T_w(z,0) = T_w^s(z), \quad T_c(z,0) = T_c^s(z)$$

and the set of PDE must have boundary contiditions, as written above, in this case:

$$c_i(0,t) = c_{i0}(t), \quad T_r(0,t) = T_{r0}(t), \quad T_c(L,t) = T_{cL}(t)$$

4 EXPERIMENTAL PART

The experimental part is mainly focused on simulation and finally practical verification of the selected simulations and control methods mentioned in the theoretical part. All methods were done first simulatively on the computer by the mathematical model and the results were then compared with those from the real model.

The following experimental part is focused on two mathematical models of chemical reactors – CSTR and tubular chemical reactors and the real model of the CSTR. The steps described in the previous chapter are applied to all these systems.

4.1 Continuous Stirred Tank Reactor

As written above, all models are divided into several parts, as it follows from the modelling procedure described in Chapter 3.1.2.

4.1.1 Description of the Model

The first model of the CSTR is schematically displayed in Figure 4.1.

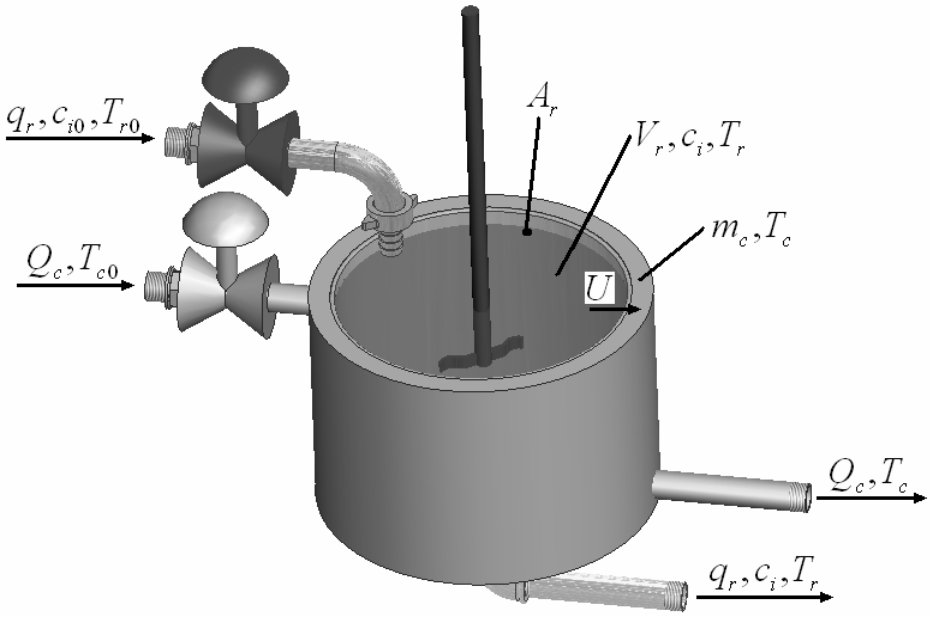


Figure 4.1 Continuous stirred tank reactor with cooling in the jacket

The reaction inside the reactor is called van der Vusse reaction and can be described by the following scheme [59]:

$$\begin{aligned} A &\xrightarrow{k_1} B \xrightarrow{k_2} C \\ 2A &\xrightarrow{k_3} D \end{aligned} \tag{4.1}$$

The mathematical description of the process is very complex and we must introduce some simplifications. In this case we expect that the reactant is perfectly mixed, all densities, heat capacities and transfer coefficients are constant throughout the reaction. In fact, they are not constant but they usually vary only in a small range, which led us to neglect this variation.

With all these simplifications we can introduce the mathematical model which is based on four material and heat balances inside the reactor described in the theoretical part (see Chapter 3.1.2).

$$\begin{aligned} \frac{dc_A}{dt} &= \frac{q_r}{V_r}\left(c_{A0} - c_A\right) - k_1 c_A - k_3 c_A^{\,2} \\ \frac{dc_B}{dt} &= -\frac{q_r}{V_r} c_B + k_1 c_A - k_2 c_B \\ \frac{dT_r}{dt} &= \frac{q_r}{V_r}\left(T_{r0} - T_r\right) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}}\left(T_c - T_r\right) \\ \frac{dT_c}{dt} &= \frac{1}{m_c c_{pc}}\left(Q_c + A_r U\left(T_r - T_c\right)\right) \end{aligned} \tag{4.2}$$

where $c_A \geq 0$, $c_B \geq 0$.

Variable t in the set of ODE (4.2) and similarly in Figure 4.1 is 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.

As can be clearly seen, this mathematical model of the reactor belongs to the class of *lumped-parameter nonlinear systems* [8] because it is described by a set of ODE. Nonlinearity can be found in reaction rates (k_j), which are described via the Arrhenius law:

$$k_j\left(T_r\right) = k_{0j} \cdot \exp\left(\frac{-E_j}{RT_r}\right), \text{for } j = 1,2,3 \tag{4.3}$$

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

The reaction heat (h_r) in Equation (4.2) is expressed as:

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B + h_3 \cdot k_3 \cdot c_A^2 \tag{4.4}$$

where h_i means reaction enthalpies.

The initial conditions for the set of ODE (4.2) are

$$c_A\left(0\right) = c_A^s, c_B\left(0\right) = c_B^s, T_r\left(0\right) = T_r^s, T_c\left(0\right) = T_c^s \tag{4.5}$$

The mathematical model of the system described by the set of ODE in Eq. (4.2) shows that this model has four state variables – $c_A(t)$, $c_B(t)$, $T_r(t)$ and $T_c(t)$.

In this step, several input variables can be used – for example 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, input and state variables

Fixed parameters of CSTR are given in Table 4.1 [59].

Table 4.1. Parameters of CSTR

Name of the parameter	Symbol and value of the parameter
Volume of the reactor	$V_r = 0.01\ m^3$
Density of the reactant	$\rho_r = 934.2\ kg.m^{-3}$
Heat capacity of the reactant	$c_{pr} = 3.01\ kJ.kg^{-1}.K^{-1}$
Weight of the coolant	$m_c = 5\ kg$
Heat capacity of the coolant	$c_{pc} = 2.0\ kJ.kg^{-1}.K^{-1}$
Surface of the cooling jacket	$A_r = 0.215\ m^2$
Heat transfer coefficient	$U = 67.2\ kJ.min^{-1}m^{-2}K^{-1}$
Pre-exponential factor for reaction 1	$k_{01} = 2.145 \cdot 10^{10}\ min^{-1}$
Pre-exponential factor for reaction 2	$k_{02} = 2.145 \cdot 10^{10}\ min^{-1}$
Pre-exponential factor for reaction 3	$k_{03} = 1.5072 \cdot 10^{8}\ min^{-1}.kmol^{-1}$
Activation energy of reaction 1 to R	$E_1/R = 9758.3\ K$
Activation energy of reaction 2 to R	$E_2/R = 9758.3\ K$
Activation energy of reaction 3 to R	$E_3/R = 8560\ K$
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 compound A	$c_{A0} = 5.1\ kmol.m^{-3}$
Input temperature of the reactant	$T_{r0} = 387.05\ K$

4.1.2 Steady-state Analysis

The theoretical background for the steady-state analysis is examined in detail in Chapter 3.1.3. The steady-state analysis for stable systems involves computing the values of state variables in time $t \rightarrow \infty$, when the changes of these variables are equal to zero. It

means that the set of ODE is solved with condition $\partial(\cdot)/\partial t = 0$. Now the set of ODE (4.2) can be rewritten to a set of nonlinear equations:

$$c_A^s = \frac{-\left(\frac{q_r}{V_r}+k_1\right) \pm \sqrt{\left(\frac{q_r}{V_r}+k_1\right)^2 - \left(4\cdot k_3 \cdot \left(-\frac{q_r}{V_r}c_{A0}\right)\right)}}{2\cdot k_3}; \qquad c_B^s = \frac{k_1 \cdot c_A^s}{k_2 + \frac{q_r}{V_r}};$$

$$T_r^s = \frac{\frac{q_r}{V_r}T_{r0} - \frac{h_r}{\rho_r \cdot c_{pr}} + \frac{U\cdot A_r}{\rho_r \cdot c_{pr}\cdot V_r}T_c^s}{\frac{q_r}{V_r} + \frac{U\cdot A_r}{\rho_r \cdot c_{pr}\cdot V_r}}; \qquad T_c^s = \frac{Q_c}{U\cdot A_r} + T_r; \tag{4.6}$$

To solve the set (4.6) a simple iteration method was used. A low value of the difference between the actual the value of the quantity and value from the previous step was chosen as a criterion for termination of the iteration process:

$$\left|T_r(i) - T_r(i-1)\right| + \left|T_c(i) - T_c(i-1)\right| < \varepsilon_{ss} \tag{4.7}$$

where (i) is an index of the actual iteration, index (i – 1) is related to the previous iteration, and ε_{ss} denotes accuracy, which was chosen in this case $\varepsilon_{ss} = 10^{-5}$.

The first graphs displayed in Figure 4.2 show the course of the computed variables through iterations.

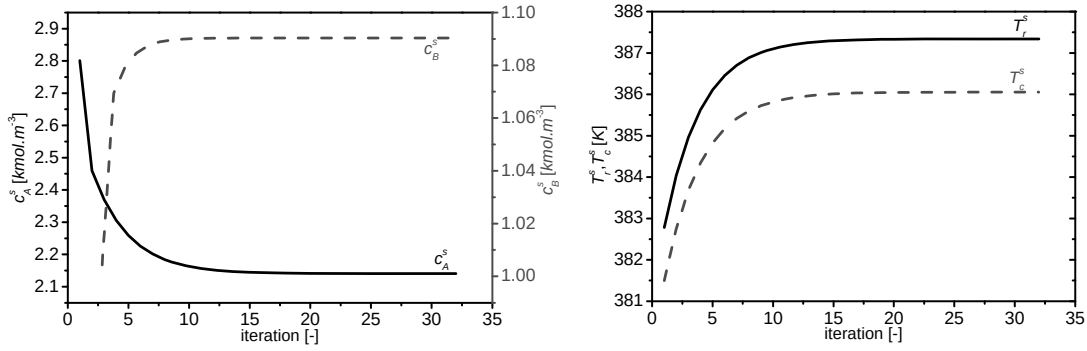


Figure 4.2 Course of iterations for concentrations c_A^s and c_B^s and temperatures T_r^s and T_c^s during the computation, CSTR

As can be clearly seen, computation leads to the solution in about thirty iterations and there is no need to further continue with the computation. Two steady-state analyses were done – for various heat removal of the cooling liquid, Q_c, in the range $Q_c = \langle -500; 500 \rangle kJ.min^{-1}$ and various volumetric flow rate of the reactant, q_r, for values $q_r = \langle 0; 0.03 \rangle m^3.min^{-1}$. The results presented in Figure 4.3 and Figure 4.4 show negative properties of the reactor – especially the course of steady-state values of concentrations c_A^s and c_B^s has highly nonlinear behaviour.

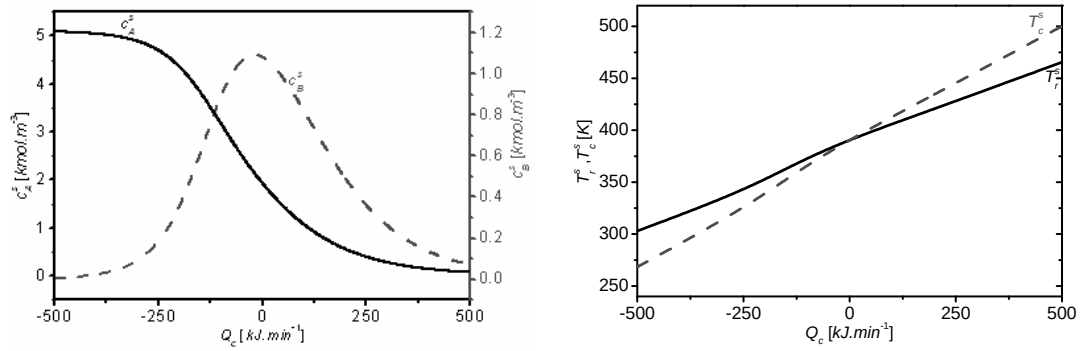


Figure 4.3 Steady-state values of concentrations c_A^s and c_B^s and temperatures T_r^s and T_c^s for various heat removal, Q_c, CSTR

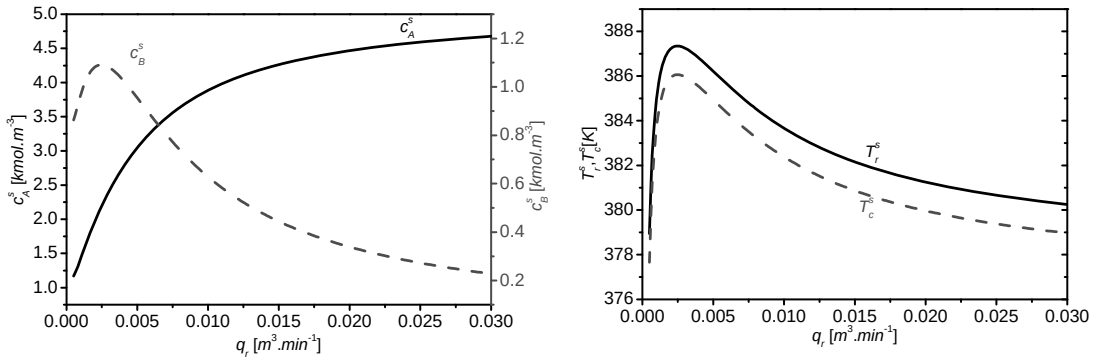


Figure 4.4 Steady-state values of concentrations c_A^s and c_B^s and temperatures T_r^s and T_c^s for various volumetric flow rate, q_r, CSTR

3D-plots of the steady-state value of concentration c_B^s and temperature T_r^s for various q_r and Q_c are in Figure 4.5.

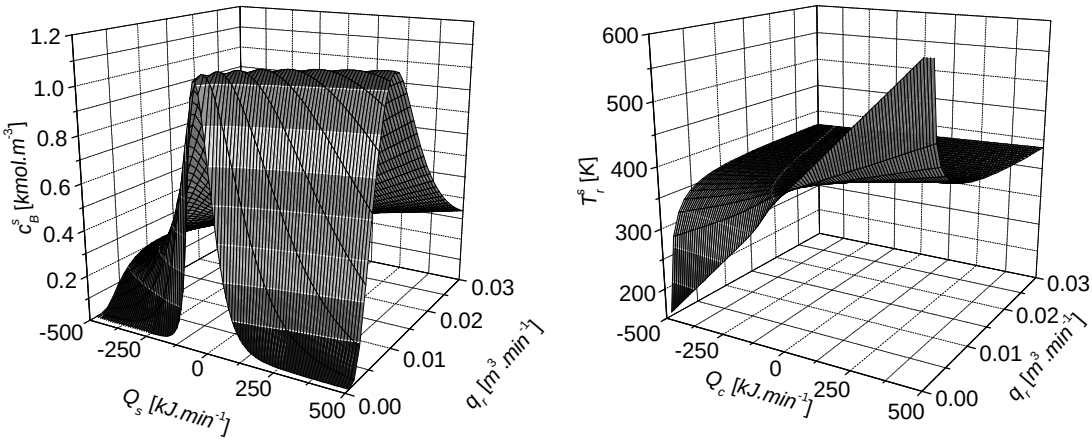


Figure 4.5 Steady-state values of the product's concentration, c_B^s, and the temperature of the reactant, T_r^s, for various heat removal, Q_c, and volumetric flow rate, q_r, CSTR

Static analysis usually results in an optimal working point. The maximum of the product's steady-state concentration, c_B^s, was chosen as a criterion for choosing an optimal working point. Concentration c_B^s has its maximum for the volumetric flow rate $q_r^s = 2.365 \cdot 10^{-3}\ m^3.min^{-1}$ and the heat removal $Q_c^s = -18.56\ kJ.min^{-1}$ – see Figure 4.3 and Figure 4.4.

4.1.3 Dynamic Analysis

The steady-state values from the previous analysis were used as input conditions for the dynamics. These values for the working point defined by the volumetric flow rate $q_r^s = 2.365 \cdot 10^{-3}\ m^3.min^{-1}$ and the heat removal $Q_c^s = -18.56\ kJ.min^{-1}$ are

$$\begin{aligned} c_A^s &= 2.1403\ kmol.m^{-3} & c_B^s &= 1.0903\ kmol.m^{-3} \\ T_r^s &= 387.34\ K & T_c^s &= 386.06\ K \end{aligned} \tag{4.8}$$

Dynamic analysis was done for various step changes of the input heat removal of the cooling liquid, Q_c, and volumetric flow rate of the reactant, q_r, which are, for better projection, recomputed to percent via

$$u(t) = \frac{Q_c(t) - Q_c^s}{Q_c^s} \cdot 100; u(t) = \frac{q_r(t) - q_r^s}{q_r^s} \cdot 100 \quad [\%] \tag{4.9}$$

Four step changes ±10% and ±20% of both input variables – the heat removal Q_c and the volumetric flow rate q_r were done. The working point from the steady-state analysis was used and these step changes can be numerically described by ΔQ_c = 3.712 (-20%), 1.856 (-20%), -1.856 (10%), -3.712 (20%) $kJ.min^{-1}$ and Δq_r = $-4.73 \cdot 10^{-4}$ (-20%), $-2.365 \cdot 10^{-4}$ (-20%), $2.365 \cdot 10^{-4}$ (10%), $4.73 \cdot 10^{-4}$ (20%) $m^3.min^{-1}$.

The fourth-order Runge-Kutta's method was used for numerical solution of the set of ODE (4.2). Although the used MATLAB program has different Runge-Kutta's methods as build-in functions, for example `ode23` (second order Runge-Kutta's method) or more common by used function `ode45` (The fourth-order Runge-Kutta's method), for our computation the easily programmed Runge-Kutta's method from chapter 3.1.4 was used. An advantage of this program is simplicity and the integration step is fixed during the computation, unlike MATLAB's build-in functions which are computed more generally and the integration step can vary according to the actual computation error. This step-variability could cause computation problems for more complex sets of ODE. Simulation time was 30 *min* and fixed integration steps h_i = 0.1 *min* were used.

Output variables $y_{1\text{-}4}$ in Figure 4.6 to Figure 4.9 illustrate the difference of variables c_A, c_B, T_r and T_c from their steady state values, which are in fact initial conditions:

$$\begin{aligned} y_1(t) &= c_A(t) - c_A^s; & y_2(t) &= c_B(t) - c_B^s; & \left[kmol.m^{-3}\right] \\ y_3(t) &= T_r(t) - T_r^s; & y_4(t) &= T_c(t) - T_c^s; & [K] \end{aligned} \tag{4.10}$$

This simplification has only one reason – all graphs start in zero and we can easily estimate time constants, gain etc.

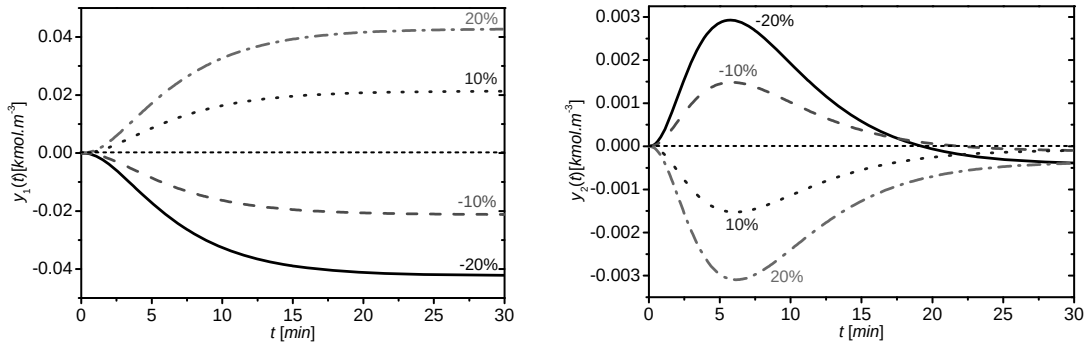


Figure 4.6 Dynamic analysis of outputs y_1 ($c_A(t) - c_A^s$) and y_2 ($c_B(t) - c_B^s$) for various step changes of the input heat removal, Q_c, CSTR

The first output responses to the step change of the input heat removal, Q_c, for outputs y_1 and y_2, which represent the differences of concentrations c_A and c_B from their steady-state values have shown that the first output, y_1, can be expressed for example by the second order transfer function. On the other hand, the output y_2 has negative properties from the control point of view – non-minimum phase behaviour and changing sign of the gain – see Figure 4.6.

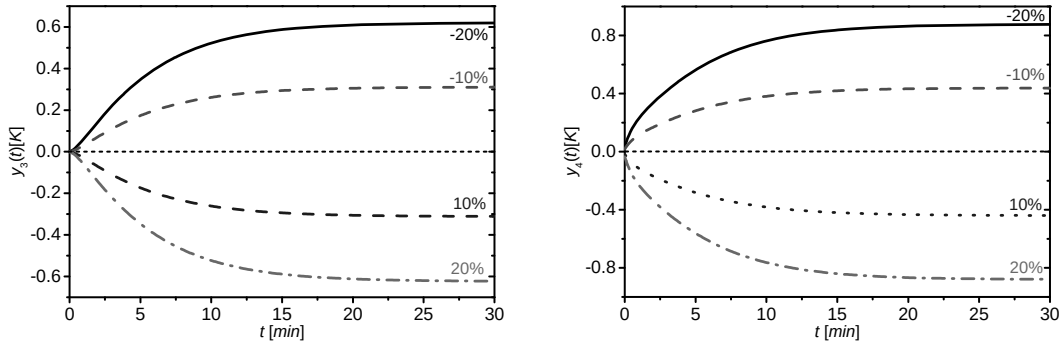


Figure 4.7 Dynamic analysis of outputs y_3 ($T_r(t) - T_r^s$) and y_4 ($T_c(t) - T_c^s$) for various step changes of the input heat removal, Q_c, CSTR

Outputs y_3 and y_4 in Figure 4.7, which represent courses of temperatures T_r and T_c related to their input values T_r^s and T_c^s, have shown that output y_3 can be approximated by the second order transfer function and the output cooling temperature in the output y_4 has a course similar to the first order transfer function.

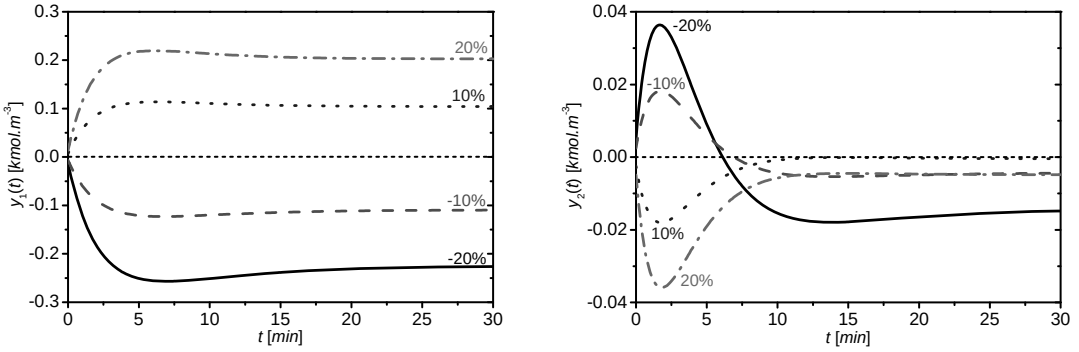


Figure 4.8 Dynamic analysis of outputs y_1 ($c_A(t) - c_A^s$) and y_2 ($c_B(t) - c_B^s$) for various step changes of the input volumetric flow rate, q_r, CSTR

The second dynamic study for various step changes of the volumetric flow rate of the reactant, q_r, presented in Figure 4.8 and Figure 4.9 shows that all outputs $y_1 - y_4$ have negative control properties similarly to output y_2 in the previous dynamic study.

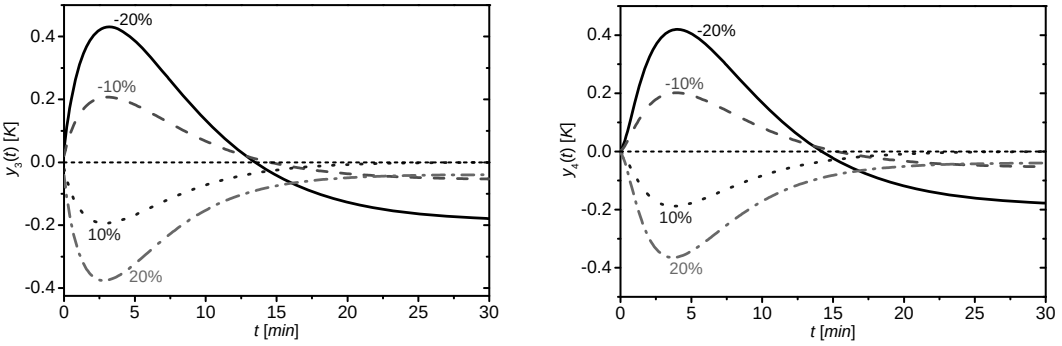


Figure 4.9 Dynamic analysis of outputs y_3 ($T_r(t) - T_r^s$) and y_4 ($T_c(t) - T_c^s$) for various step changes of the input flow rate, q_r, CSTR

The dynamic analysis shows the response of output variables to the step change of the input quantity. This was mainly done for control purposes. It shows output properties and helps with the choice of the appropriate control strategy.

4.1.4 Simulation of Control

The first control strategy used in the simulation part is Adaptive control described in detail in Chapter 3.2.1.

The Adaptive control used in this work is based on an choice of the appropriate External Linear Model (ELM) of the originally nonlinear process parameters of which are estimated recursively during the control. The parameters of the controllers are recomputed according to the estimated parameters in every step too. The polynomial approach with the pole-placement method and two control configurations with one degree-of-freedom (1DOF) and two degrees-of-freedom (2DOF) were used for design of the controller.

Based on the dynamic study, the step change of the heat removal of the cooling, Q_c, was chosen as an input (control) variable $u(t)$ and the temperature of the reactant, T_r, again related to its initial condition (steady-state value) was used as an output (controlled) variable $y(t)$, i.e.

$$u(t) = \frac{Q_c(t) - Q_c^s}{Q_c^s} \cdot 100\,[\%];\; y(t) = T_r(t) - T_r^s\,[K] \tag{4.11}$$

The output $y(t)$ can be represented by the second order transfer function with relative order one:

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0} \tag{4.12}$$

The parameters of polynomials $a(s)$ and $b(s)$ in (4.12) are estimated recursively during the control with the use of RLS method with changing exponential forgetting, where forgetting factor λ_1 is recomputed in every step via Equation (3.65). The initial values are: $K = 0.001$ and parameters $\gamma(0) = 0$, $\varepsilon(0) = 0$.

The working point and initial values for identification are shown in Table 4.2.

Table 4.2 Working point and parameters of the identification used for the control, CSTR

Name of the parameter	Symbol and value of the parameter
Input concentration of compound A Input temperature of the reactant Input volumetric flow rate of the reactant Input heat removal of cooling	$c_{A0} = 5.1\ kmol.m^{-3}$ $T_{r0} = 387.05\ K$ $q_r^s = 2.365 \cdot 10^{-3}\ m^3.min^{-1}$ $Q_c^s = -18.56\ kJ.min^{-1}$
Starting vector of parameters	$\boldsymbol{\theta}_\delta(0) = [0.1, 0.1, 0.1, 0.1]^T$
Starting covariance matrix	$\mathbf{P}(0) = \begin{bmatrix} 1 \cdot 10^6 & 0 & 0 & 0 \\ 0 & 1 \cdot 10^6 & 0 & 0 \\ 0 & 0 & 1 \cdot 10^6 & 0 \\ 0 & 0 & 0 & 1 \cdot 10^6 \end{bmatrix}$

The quality of control was evaluated by the quality criteria S_u and S_y computed for a time interval as

$$S_u = \sum_{i=2}^{N} \left(u(i) - u(i-1)\right)^2 [-]; \quad S_y = \sum_{i=1}^{N} \left(w(i) - y(i)\right)^2 [-], \text{ for } N = \frac{T_f}{T_v} \tag{4.13}$$

where T_f is time of simulation – in this case $T_f = 450\ min$.

The best results will be compared in the last part of this chapter. The sampling period T_v = 0.3 *min* is common for all studies and the course of the reference signal (wanted value), $w(t)$, is:

$$\begin{aligned} w(t) &= 2 \cdot [1 - \exp(-0.1 \cdot t)]\ K && \text{for } t \in \langle 0; 150 \rangle\ min \\ w(t) &= -1\ K && \text{for } t \in (150; 300)\ min \\ w(t) &= 1\ K && \text{for } t \in \langle 300; 450 \rangle\ min \end{aligned} \tag{4.14}$$

The action value (input signal) is limited due to technological reasons $u(t)$ = <-75;+75> % of Q_c^s. Several simulation studies were done and some of them will be presented in the next chapters and figures.

ADAPTIVE CONTROL WITH POLE-PLACEMENT METHOD

The first adaptive controller uses spectral factorization to design a stable polynomial $d(s)$ on the right side of Diophantine equations (3.81), (3.92) and (3.94).

The controller has the *1DOF configuration* which means that it has only in the feedback part (see Figure 3.2). The transfer function of the controller $Q(s)$ (3.82), with the condition that reference signal $w(t)$ and disturbance $v(t)$ are chosen from the range of the step functions, has form

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)} \tag{4.15}$$

where the parameters of polynomials $q(s)$ and $\tilde{p}(s)$ are computed from the Diophantine equation

$$a(s) \cdot s \cdot \tilde{p}(s) + b(s) \cdot q(s) = d(s) \tag{4.16}$$

by *the method of comparison of the coefficients*.

The degrees of polynomials $d(s)$, $q(s)$ and $\tilde{p}(s)$ are then, according to (3.84), (3.87), (3.88) and (4.12),

$$\begin{aligned} &\deg d(s) = \deg a(s) + \deg \tilde{p}(s) + 1 = 2 + 1 + 1 = 4 \\ &\deg q(s) = \deg a(s) = 2 \\ &\deg \tilde{p}(s) \geq \deg a(s) - 1 \Rightarrow \deg \tilde{p}(s) = 2 - 1 = 1 \end{aligned} \tag{4.17}$$

The transfer function of the controller (4.15) is then

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s \cdot (s + p_0)} \tag{4.18}$$

Polynomial $d(s)$ on the right side of the Diophantine equation (3.81) can be divided into two polynomials: $d(s) = m(s) \cdot n(s)$ (see (3.109)), where polynomial $n(s)$ is computed by the spectral factorization of polynomial $a(s)$:

$$n^*(s) \cdot n(s) = a^*(s) \cdot a(s) \tag{4.19}$$

The degree of polynomial $n(s)$ is equal to $\deg a(s)$, i.e.

$$n(s) = s^2 + n_1 s + n_0 \Rightarrow n_0 = \sqrt{a_0^2}\,;\; n_1 = \sqrt{a_1^2 + 2n_0 - 2a_0} \tag{4.20}$$

The second part of polynomial $d(s)$, stable polynomial $m(s)$ was chosen as

$$m(s) = (s + \alpha_i)^{\deg d - \deg n} = (s + \alpha_i)^2 \tag{4.21}$$

which results in one double root where $\alpha_i > 0$.

On the contrary, *control configuration with two degrees-of-freedom – 2DOF* (Figure 3.3) has controller divided into two parts – the feedback part with transfer function $Q(s)$ and the feedforward part with transfer function $R(s)$, which are for step functions of reference signal $w(t)$ and disturbance $v(t)$:

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)},\; \tilde{R}(s) = \frac{r(s)}{s \cdot \tilde{p}(s)} \tag{4.22}$$

where parameters of polynomials $\tilde{p}(s)$, $q(s)$ and $r(s)$ are computed by the method of comparison of the coefficients from the set of two Diophantine equations (3.94) and (3.92):

$$\begin{aligned} a(s) \cdot s \cdot \tilde{p}(s) + b(s) q(s) &= d(s) \\ t(s) \cdot s + b(s) r(s) &= d(s) \end{aligned} \tag{4.23}$$

where $t(s)$ is only additional polynomial used for solution and it is not used in transfer functions.

The degrees of polynomials $\tilde{p}(s)$, $q(s)$, $r(s)$ and $d(s)$ are computed via (3.96) to (3.105):

$$\begin{aligned}
&\deg q(s) = \deg a(s) = 2 \\
&\deg p(s) = \deg a(s) - 1 = 2 - 1 = 1 \\
&\deg r(s) = 0 \\
&\deg d(s) = 2\deg a(s) = 2 \cdot 2 = 4 \\
&\deg t(s) = \deg d(s) - 1 = 4 - 1 = 3
\end{aligned} \tag{4.24}$$

and transfer functions (4.22) are

$$\begin{aligned}
\tilde{Q}(s) &= \frac{q(s)}{s \cdot \tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s \cdot (s + p_0)} \\
\tilde{R}(s) &= \frac{r(s)}{s \cdot \tilde{p}(s)} = \frac{r_0}{s \cdot (s + p_0)}
\end{aligned} \tag{4.25}$$

The choice of the stable polynomial $d(s)$ is similar as for 1DOF control configuration. Both 1DOF and 2DOF control configurations δ-ELM were used.

The estimated output is recomputed recursively from differential equation

$$y_\delta(k) = \boldsymbol{\theta}_\delta^T(k) \cdot \boldsymbol{\varphi}_\delta(k-1) \tag{4.26}$$

where the vector of the parameters, $\boldsymbol{\theta}_\delta$, and the data vector, $\boldsymbol{\varphi}_\delta$, are

$$\boldsymbol{\theta}_\delta(k) = \left[a_1', a_0', b_1', b_0'\right]^T; \quad \boldsymbol{\varphi}_\delta(k-1) = \left[-y_\delta(k-1), -y_\delta(k-2), u_\delta(k-1), u_\delta(k-2)\right]^T \tag{4.27}$$

and

$$\begin{aligned}
&y_\delta(k) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_v^2} \\
&y_\delta(k-1) = \frac{y(k-1) - y(k-2)}{T_v} \qquad u_\delta(k-1) = \frac{u(k-1) - u(k-2)}{T_v} \\
&y_\delta(k-2) = y(k-2) \qquad u_\delta(k-2) = u(k-2)
\end{aligned} \tag{4.28}$$

Three simulation studies were done for different values of parameter α_i = 0.05, 0.1 and 0.4, which represent the position of the double root.

Figure 4.10, which represents the course of the input variable, $u(t)$, the reference signal, $w(t)$, and the output variable, $y(t)$, for the control configuration with 1DOF, clearly shows that the output response is quicker with increasing value of parameter α_i. On the other hand, there can be some overshoots of the output variable and the course of the input variable, $u(t)$, is not so smooth for bigger values of α_i.

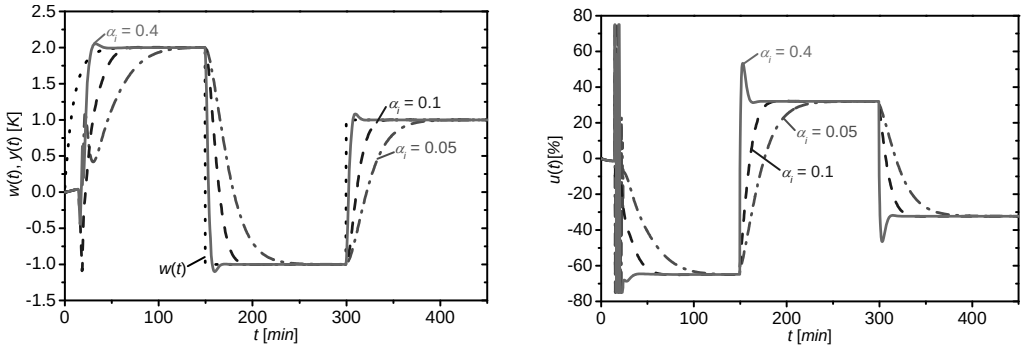


Figure 4.10 The course of $y(t)$, $w(t)$ and $u(t)$ for different position of the parameter α_i = 0.05, 0.1 and 0.4, 1DOF, pole-placement method, δ-ELM, CSTR

The course of identified parameters a'_0, a'_1, b'_0 and b'_1 in Figure 4.11 shows that the used recursive identification has no problem with parameter estimation during the control except for the very beginning, where the apriory information about the system is insufficient. It is desirable to include some forgetting factor in the identification because the estimated parameters without forgetting correspond to the average values and all input-output samples have the same weight for estimation.

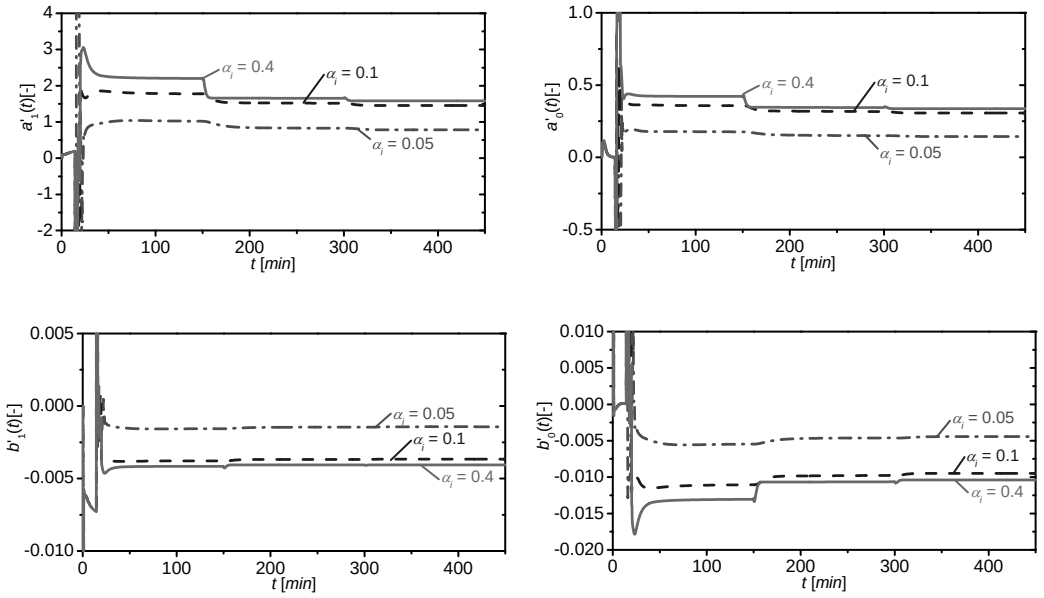


Figure 4.11 The course of identified parameters a'_0, a'_1, b'_0 and b'_1 during the control, 1DOF, pole-placement method, δ-ELM, CSTR

Figure 4.12 shows the results for 2DOF configuration. As can be seen, the results are similar as for 1DOF – the increasing value of parameter α_i mainly affects overshoots and the speed of control.

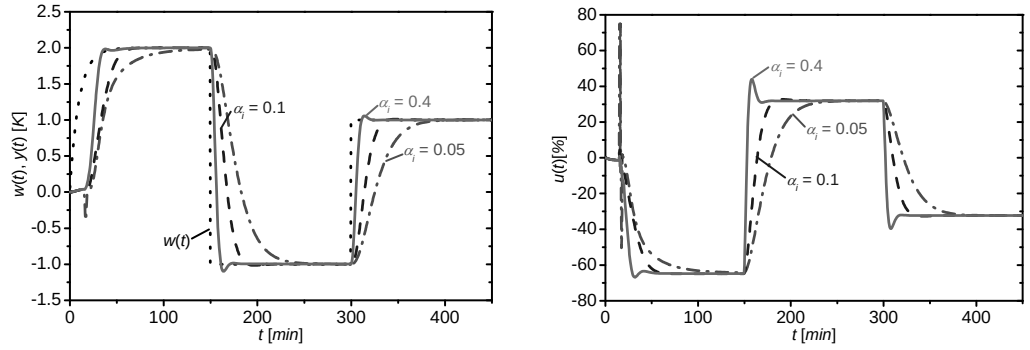


Figure 4.12 The course of $y(t)$, $w(t)$ and $u(t)$ for different position of the parameter α_i = 0.05, 0.1 and 0.4, 2DOF, pole-placement method, δ-ELM, CSTR

The comparison of control results with 1DOF and 2DOF configuration in Figure 4.13 shows the main advantage of the 2DOF control configuration – lower overshoots and smoother course of the action value, which is an important criterion too. The change of the action value can be represented by the valve turn and rapid changes on the valve can destroy it.

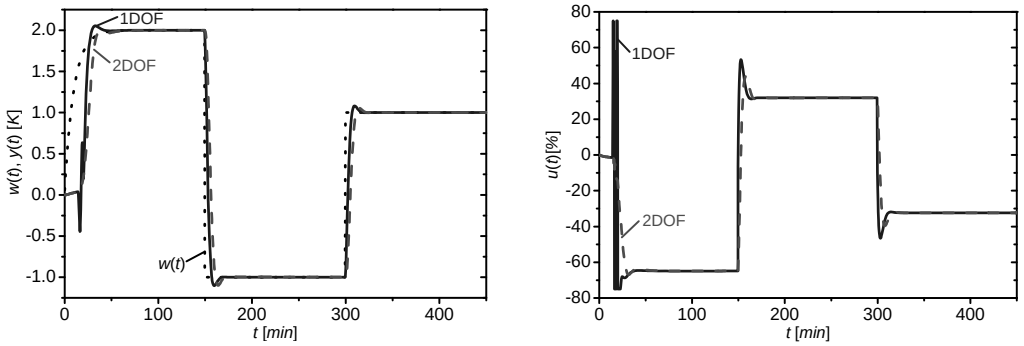


Figure 4.13 The course of $y(t)$, $w(t)$ and $u(t)$ for 1DOF and 2DOF, pole-placement method, $\alpha_i = 0.4$, δ-ELM, CSTR

Table 4.3 presents the results of control from the control quality point of view according to Equation (4.13). The best results (in the table in bold) are in this case for the parameter $\alpha_i = 0.4$.

Table 4.3 The control quality criteria S_u, S_y for pole-placement method, δ-ELM, CSTR

	1DOF		**2DOF**	
	S_u[-]	S_y[-]	S_u[-]	S_y[-]
$\alpha_i = 0.05$	60457	975.19	23878.00	1056.20
$\alpha_i = 0.1$	32151	590.24	352.55	677.99
$\alpha_i = 0.4$	**62933**	**198.81**	**1059.00**	**314.62**

As written in the theoretical part, the nominated adaptive controller can deal with disturbance attenuation, which is proved in Figure 4.14. The simulation was done for

1DOF control configuration and various values of parameter α_i = 0.05, 0.1 and 0.4, the sampling period was T_v = 0.3 *min*, the simulation time 500 *min* with one step change $w(t) = 2 \cdot [1 - \exp(-0.1 \cdot t)]\ K$. Tree types of disturbances, two in the input and one on the output, are injected to the system during this time:

- $v_1(t)$ = +3% step change of the input concentration c_{A0} for time $t \in \langle 150; 500 \rangle\ min$
- $v_2(t)$ = -0.5 *K* step change of the input temperature T_{r0} for time $t \in \langle 250; 500 \rangle\ min$
- $v_3(t)$ = 0.5 *K* step change of the output temperature T_r for time $t \in \langle 400; 500 \rangle\ min$

As can be seen from Figure 4.14, presence of the integration part in the controller ensures full attenuation of the disturbances on the input or output, respectively. All three disturbances are suppressed by the used adaptive controller with 1DOF control configuration. The only difference is in the speed of control and disturbance attenuation. The response with the lowest value of α_i = 0.05 results in the slowest course of the output variable and the disturbance is suppressed slowly, while the biggest value α_i = 0.4 represses the influence of the disturbance faster but with a small overshoot of the output variable at the very beginning.

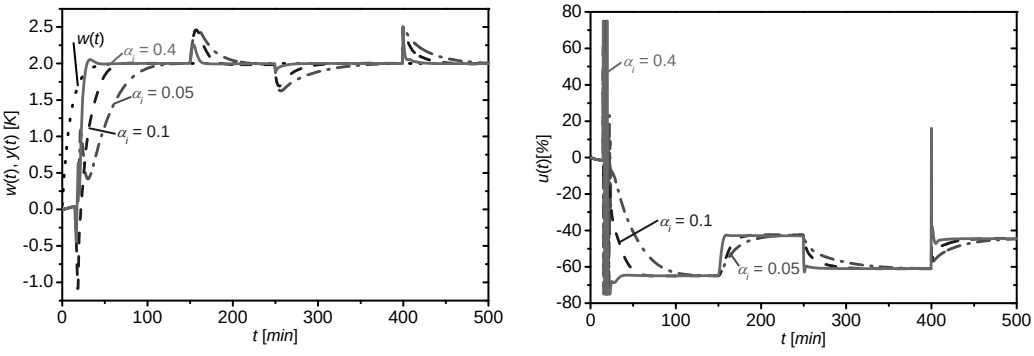


Figure 4.14 The course of $y(t)$, $w(t)$ and $u(t)$ for three disturbances and more values of the parameter α_i, 1DOF, pole-placement method, δ-ELM, CSTR

The values of the quality indicate that the best results were reached for the $\alpha_i = 0.4$, as also clear from the previous graph.

Table 4.4 The control quality criteria S_u, S_y for pole-placement method, δ-ELM, CSTR

	S_u[-]	S_y[-]
$\alpha_i = 0.05$	60561	297.98
$\alpha_i = 0.1$	32221	247.82
$\alpha_i = 0.4$	**65938**	**116.03**

ADAPTIVE CONTROL WITH LQ APPROACH

The disadvantage of the pole-placement method is that it is an intuitive method and there is no general role for the choice of parameter α_i. This disadvantage should be overcome, for example, by the use of Linear Quadratic (LQ).

This method is based on minimization of the quadratic criterion J_{LQ} in (3.112), which, in this concrete example, means that polynomial $d(s)$ on the right side of Diophantine equations (3.81), (3.92) and (3.94) is $d(s) = g(s) \cdot n(s)$. Polynomials $n(s)$ and $g(s)$ are computed from spectral factorization (3.114) which means that the coefficients of the polynomials $n(s)$ and $g(s)$ are calculated as

$$g_0 = \sqrt{\mu_{LQ} b_0^2},\ g_1 = \sqrt{2g_0g_2 + \varphi_{LQ}a_0^2 + \mu b_1^2},\ g_2 = \sqrt{2g_1g_3 + \varphi_{LQ}\left(a_1^2 - 2a_0\right)},\ g_3 = \sqrt{\varphi_{LQ}},$$
$$n_0 = \sqrt{a_0^2},\ n_1 = \sqrt{2n_0 + a_1^2 - 2a_0} \tag{4.29}$$

Transfer functions of the controller for both 1DOF and 2DOF control configurations are similar as in Equation (4.22). The degrees of the polynomials $d(s)$, $q(s)$, $r(s)$ and $\tilde{p}(s)$ are

$$\begin{aligned}
&\deg d(s) = \deg\left(g(s)\cdot n(s)\right) = 2\deg a(s) + 1 = 2\cdot 2 + 1 = 5\\
&\deg q(s) = \deg a(s) = 2\\
&\deg \tilde{p}(s) \geq \deg a(s) - 1 = 2\\
&\deg r(s) = 0
\end{aligned} \tag{4.30}$$

and transfer functions (4.22) are

$$\begin{aligned}
\tilde{Q}(s) &= \frac{q(s)}{s\cdot\tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s\cdot\left(s^2 + p_1 s + p_0\right)}\\
\tilde{R}(s) &= \frac{r(s)}{s\cdot\tilde{p}(s)} = \frac{r_0}{s\cdot\left(s^2 + p_1 s + p_0\right)}
\end{aligned} \tag{4.31}$$

The parameters of polynomials $q(s)$, $r(s)$ and $\tilde{p}(s)$ in (4.31) are then computed again by *the method of parameters comparison*.

The ELM was chosen from the range of δ-models and simulations were done for more values of weighting factor ϕ_{LQ}, the second weighting factor was set to $\mu_{LQ} = 1$; results are shown in the following figures.

The course of the output variable, $y(t)$, and the input variable $u(t)$ for 1DOF control configuration is shown in Figure 4.15.

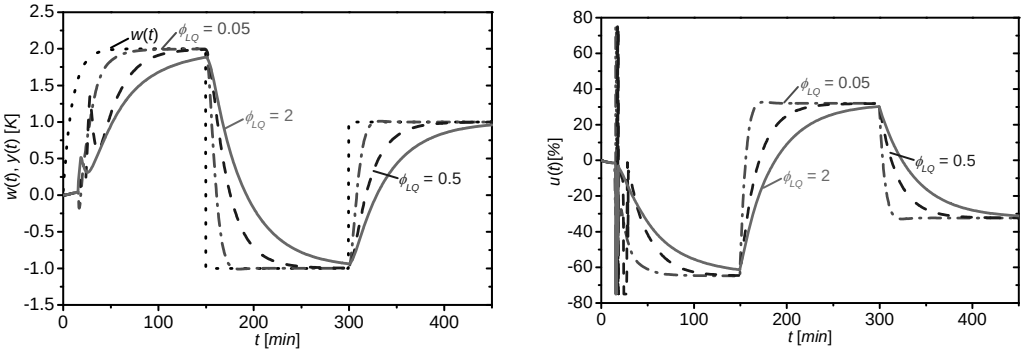


Figure 4.15 The course of $y(t)$, $w(t)$ and $u(t)$ for different weighting factor ϕ_{LQ} = 0.05, 0.5 and 2, 1DOF, LQ method, δ-ELM, CSTR

As can be seen, the speed of control is quicker with a decreasing value of weighting factor ϕ_{LQ}. Control responses have minimal overshoots at the very beginning of the control and there is no other overshoot for the next step changes for this concrete case.

The course of identified parameters a'_0, a'_1, b'_0 and b'_1 in Figure 4.16 indicates problems at the very beginning because of initial adaptation but the identification after 50 minutes has no computational problems.

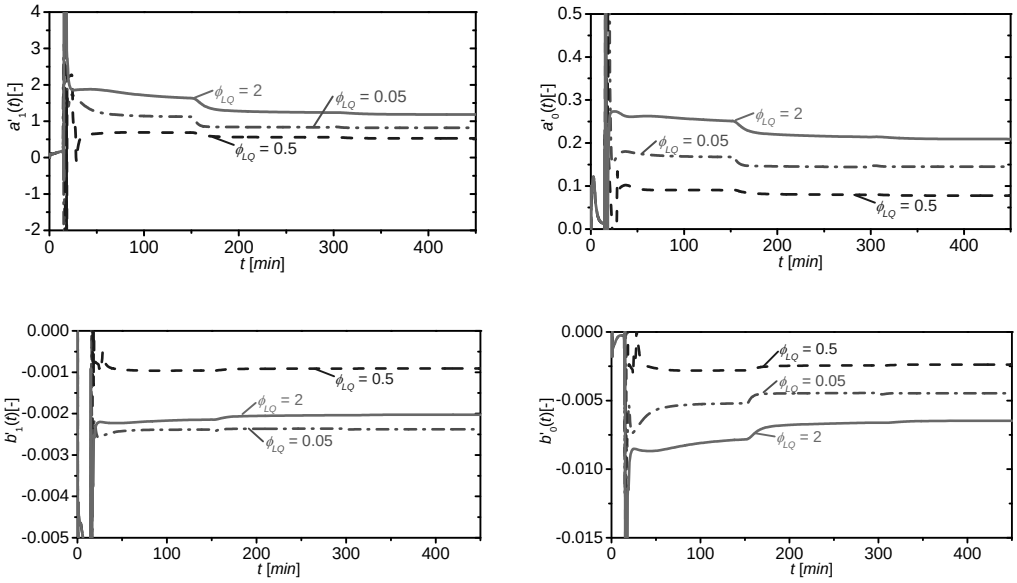


Figure 4.16 The course of identified parameters a'_0, a'_1, b'_0 and b'_1 during control, 1DOF, LQ method, δ-ELM, CSTR

The 2DOF control configuration displayed in Figure 4.17 shows similar results as in the previous one. The controller has problems only for weighting factor $\phi_{LQ} = 0.05$ at the beginning and there are some small overshoots after next step changes.

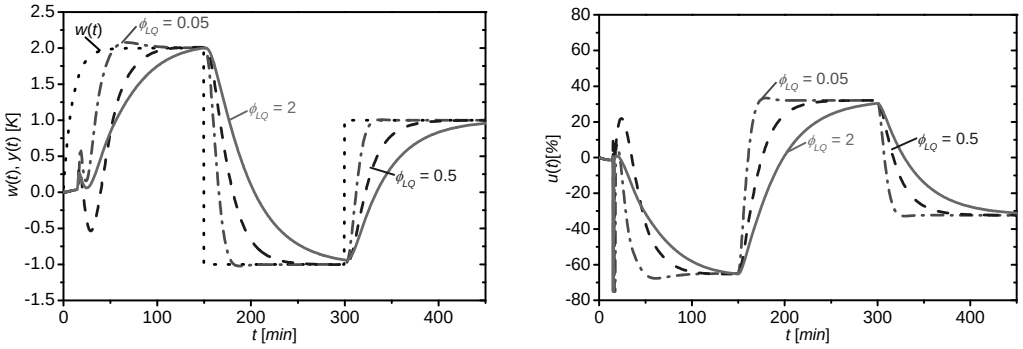


Figure 4.17 The course of $y(t)$, $w(t)$ and $u(t)$ for different weighting factor ϕ_{LQ} = 0.05, 0.5 and 2, 2DOF, LQ method, δ-ELM, CSTR

Finally Figure 4.18 compares control results with 1DOF a 2DOF control configurations for ϕ_{LQ} = 0.5. The courses show similar results except for starting 100 *min*, where 1DOF has small problems with identification, which can be clearly seen in the course of input variable $u(t)$ in the right-hand side graph.

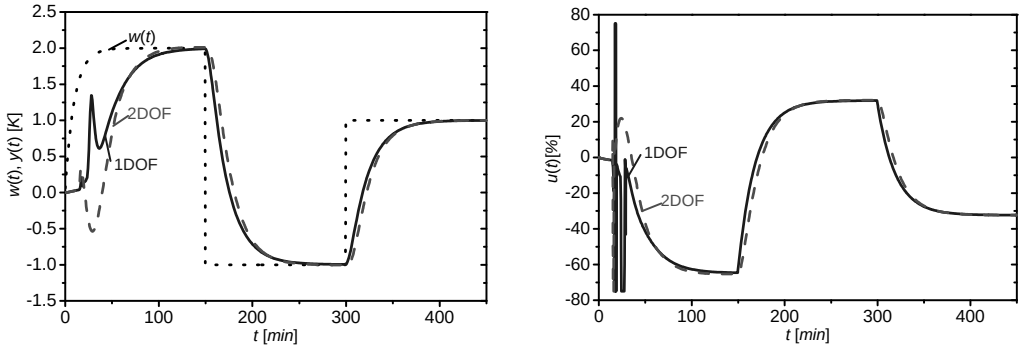


Figure 4.18 The course of $y(t)$, $w(t)$ and $u(t)$ for 1DOF and 2DOF, LQ method, ϕ_{LQ} = 0.5, δ-ELM, CSTR

Table 4.5 shows the values of criteria S_u and S_y for different values of weighting factor ϕ_{LQ}. The best results are reached for ϕ_{LQ} = 0.05 (in bold).

Table 4.5 The control quality criteria S_u and S_y for LQ method, δ-ELM, CSTR

	1DOF		2DOF	
	S_u[-]	S_y[-]	S_u[-]	S_y[-]
ϕ_{LQ} = 0.05	**20824**	**433.9**	**17260**	**628.1**
ϕ_{LQ} = 0.5	104220	860.0	13085	1318.2
ϕ_{LQ} = 2	13116	1256.6	21272	1647.5

ADAPTIVE CONTROL WITH CONTINUOUS-TIME ELM

The third control analysis was done for Continuous-Time (CT) ELM instead of δ-models. The difference equation for transfer function of the ELM (4.12) is

$$y^{(2)}(t) + a_1 y^{(1)}(t) + a_0 y(t) = b_1 u^{(1)}(t) + b_0 u(t) \tag{4.32}$$

and filtered variables u_f and y_f are, according to Equation (3.31):

$$\begin{aligned} y_f^{(2)}(t) + c_1 y_f^{(1)}(t) + c_0 y_f(t) &= y(t) \\ u_f^{(2)}(t) + c_1 u_f^{(1)}(t) + c_0 u_f(t) &= u(t) \end{aligned} \tag{4.33}$$

where parameters c_1 and c_0 were chosen 1.4 and 0.49, respectively. The choice of these parameters was done after several simulation experiments. There is no general rule for the choice of these parameters, but they must be lower than parameters of the ELM.

The identification part then solves the differential equation (4.32) in the vector form

$$y_f^{(n)}(t_k) = \boldsymbol{\theta}^T(t_k) \cdot \boldsymbol{\varphi}(t_k) \tag{4.34}$$

where data vector, $\boldsymbol{\varphi}$, and vector of parameters, $\boldsymbol{\theta}$, are:

$$\begin{aligned}\boldsymbol{\varphi}(t_k) &= \left[-y_f(t_k), -y_f^{(1)}(t_k), u_f(t_k), u_f^{(1)}(t_k)\right]^T \\ \boldsymbol{\theta}(t_k) &= \left[a_0, a_1, b_0, b_1\right]^T\end{aligned} \tag{4.35}$$

and t_k is discrete time moment $t_k = k \cdot T_v$ for k = 0,1,2,… and T_v as the sampling period.

Control system configurations with 1DOF and 2DOF are computed similarly to previous cases. The stable polynomial on the right side of Diophantine equations (4.16) and (4.23) was designed by the pole-placement method with spectral factorization similar as like in Part I of this chapter.

The simulation study for different values of parameter α_i = 0.05, 0.1 and 0.4 was done and the results are shown in the following graphs.

The course of output and input variables for both 1DOF and 2DOF control configurations in Figure 4.19 and Figure 4.21 show that the output variable, $y(t)$, reaches the reference signal, $w(t)$, faster with increasing value of parameter α_i. This quick response results in overshoots of the output variable and rapid changes of the input variable, which are bad attributes of the high value of α_i.

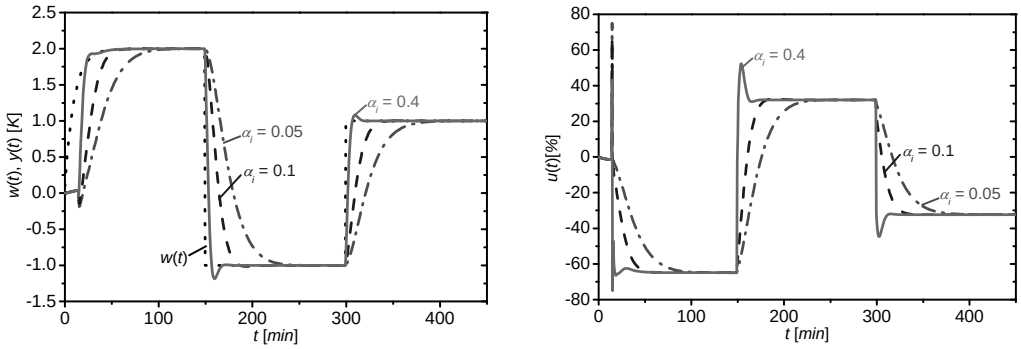


Figure 4.19 The course of $y(t)$, $w(t)$ and $u(t)$ for different position of parameter α_i = 0.05, 0.1 and 0.4, 1DOF, pole-placement method, CT ELM, CSTR

The recursive identification with exponential forgetting works properly from approximately 50 *min* after start, when the system has enough information about the system – see Figure 4.20. The course of the identified parameters a_0, a_1, b_0 and b_1 after this time is relatively stable.

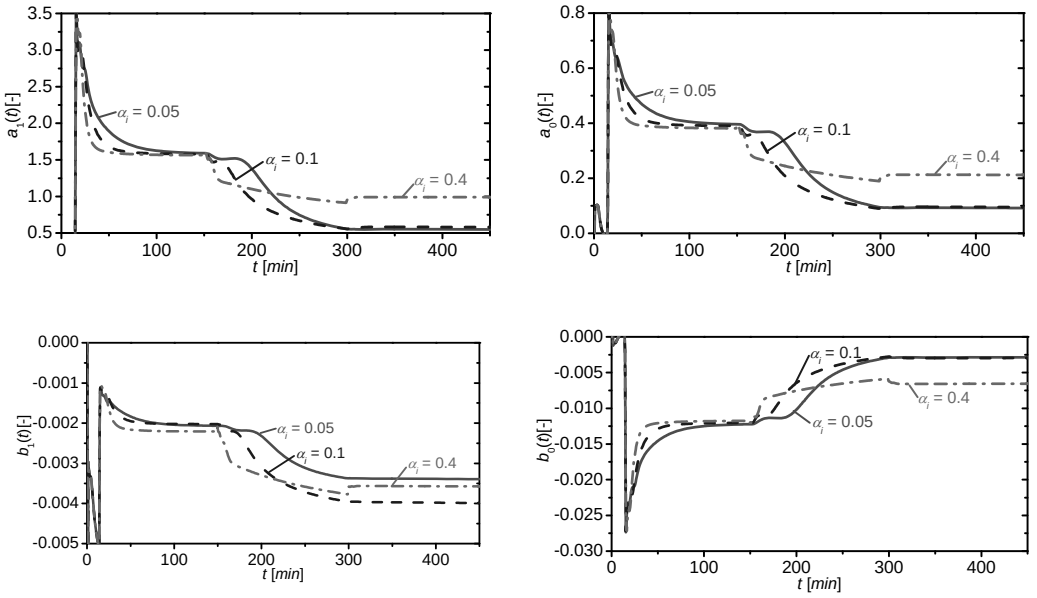


Figure 4.20 The course of identified parameters a_0, a_1, b_0 and b_1 during control, 1DOF, pole-placement method, CT ELM, CSTR

The course of the output variable for parameter $\alpha_i = 0.1$ has problems after the second time step, which may be caused by computation problems – see the blue dashed line in Figure 4.21.

Table 4.6 presents the results of the simulation of control with the continuous-time ELM. It can be said that setting of the controller with parameter $\alpha_i = 0.4$ has the best results from the viewpoint of control quality criteria S_u and S_y.

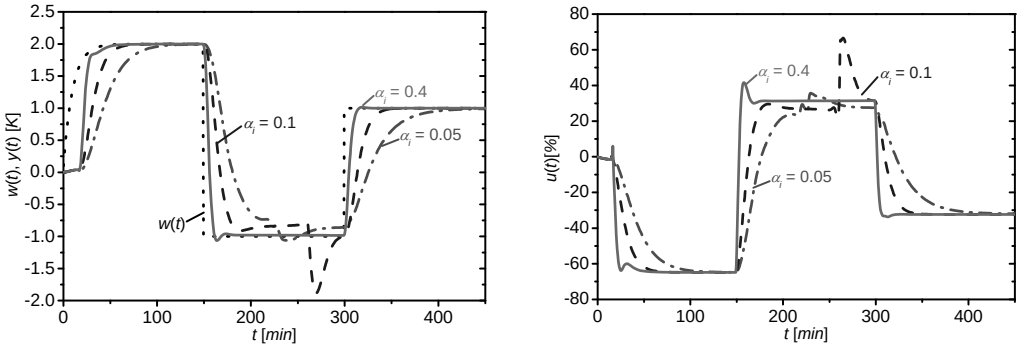


Figure 4.21 The course of $y(t)$, $w(t)$ and $u(t)$ for different positions of parameter α_i = 0.05, 0.1 and 0.4, 2DOF, pole-placement method, CT ELM, CSTR

Table 4.6 The quality criteria S_u and S_y for pole-placement method, CT ELM, CSTR

	1DOF		**2DOF**	
	S_u[-]	S_y[-]	S_u[-]	S_y[-]
α_i = 0.05	1289.67	1029.47	106.14	1259.50
α_i = 0.1	10533.92	540.46	287.30	777.53
α_i = 0.4	**14452.63**	**161.56**	**13307.10**	**313.40**

Figure 4.22 and Figure 4.23 compare control results for 1DOF and 2DOF configurations, the δ-ELM presented in Part I. and the continuous-time ELM from this section. As can be seen, the main difference is at the very beginning, where the course for the CT ELM has a smoother course and the changes of the input variable are not so quick. The differences are not very significant in this concrete example, but other simulations have shown benefits of CT ELM. Disadvantage of CT ELM can be found in the computation demanding.

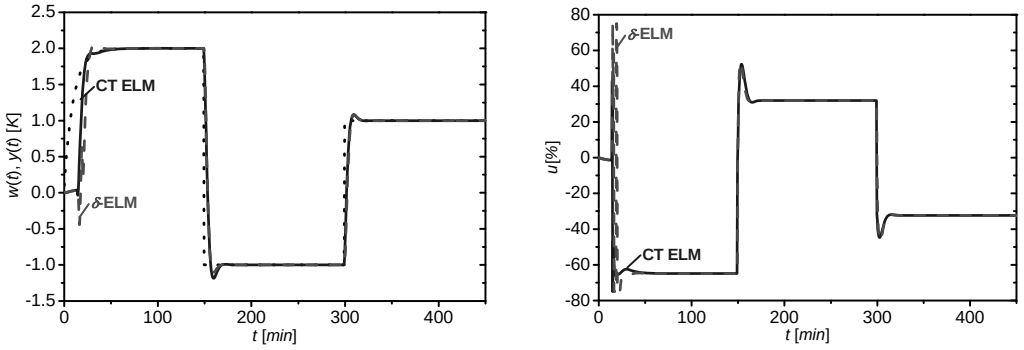


Figure 4.22 The course of $y(t)$, $w(t)$ and $u(t)$ for δ-ELM and CT ELM, pole-placement method, $\alpha_i = 0.4$, 1DOF control configuration, CSTR

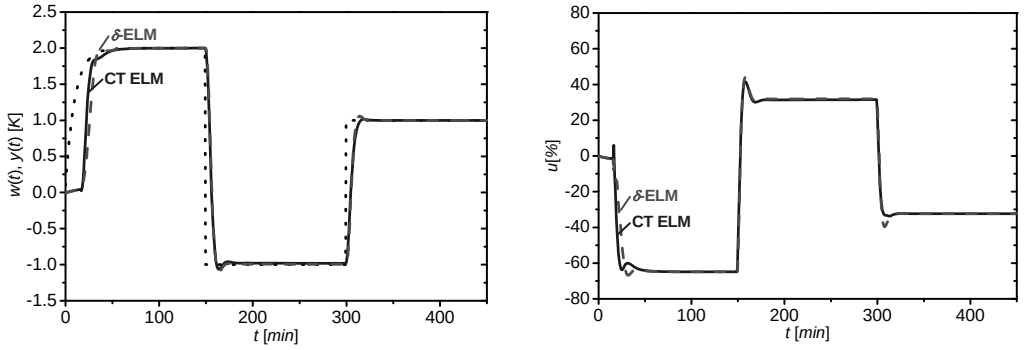


Figure 4.23 The course of $y(t)$, $w(t)$ and $u(t)$ for δ-ELM and CT ELM, pole-placement method, $\alpha_i = 0.4$, 2DOF control configuration, CSTR

The values of coefficients S_u and S_y Table 4.7 show better control results for the CT ELM, which is in accordance with the previous graphs.

Table 4.7 The control quality criteria S_u and S_y for $\delta-$ and CT ELM, $\alpha_i = 0.4$, CSTR

	1DOF		**2DOF**	
	S_u[-]	S_y[-]	S_u[-]	S_y[-]
δ–ELM	62933	198.81	1059	314.62
CT ELM	14452	161.56	13307	313.40

PREDICTIVE CONTROL

The last simulation study on this type of chemical reactor was done for the Generalized Predictive Control (GPC) presented theoretically in Chapter 3.2.2.

The goal of the GPC is minimization of the cost function J_{GPC} represented by Equation (3.120). The sampling period was $T_v = 0.3$ *min* in this case, the prediction horizon starts at $N_1 = 0$, ends in $N_2 = 49$ steps ahead and the length of the manipulation horizon is $N_u = 10$ steps.

Weighting factors $\delta_u(j)$ and $\lambda_u(j)$ are constant throughout the whole prediction horizon, and $\delta_u = 1$. The simulation study was done for different value, of the weighting factor $\lambda_u = 0.05$, 0.5 and 2.

The system is expected to be linear and is described by the discrete-time transfer function

$$G\left(z^{-1}\right) = \frac{B\left(z^{-1}\right)}{A\left(z^{-1}\right)} \tag{4.36}$$

Parameters of polynomials $A(z^{-1})$ and $B(z^{-1})$ can be derived from the identification presented above.

The continuous-time ELM $G(s)$ from the identification

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0} = \frac{-0.0063s - 0.0151}{s^2 + 1.5950s + 0.4856} \tag{4.37}$$

has, for the used sampling period $T_v = 0.3$ *min* in the discrete-time, form

$$G\left(z^{-1}\right) = \frac{-0.0021z^{-1} + 0.0010z^{-2}}{1 - 1.5851z^{-1} + 0.6197z^{-2}} \tag{4.38}$$

and zero mean white noise $e(t)$ is not take into account.

The control results presented in Figure 4.24 show that the course of the output temperature is faster with increasing value of weighting factor λ_u but some small overshoots may occur for the highest value, $\lambda_u = 2$. The ideal value of this factor seems to be the middle one, i.e. $\lambda_u = 0.5$.

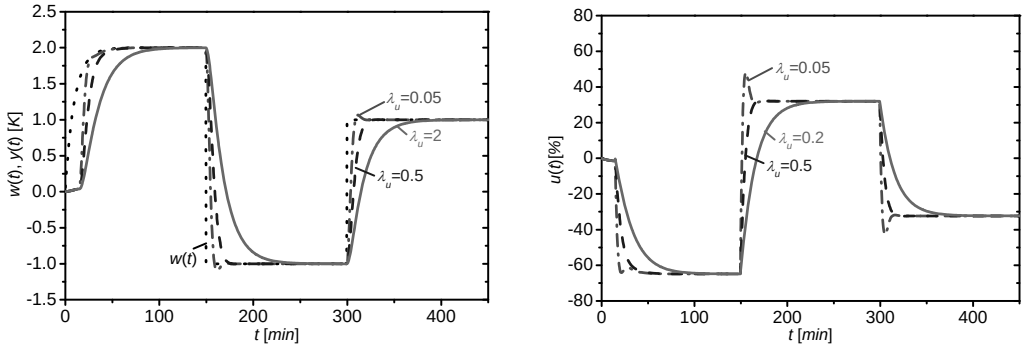


Figure 4.24 The course of $y(t)$, $w(t)$ and $u(t)$ for predictive control and different values of $\lambda_u = 0.05$, 0.5 and 2, CSTR

Table 4.8 presents the results of control from the control criterion's point of view. As can be seen, value $\lambda_u = 2$ is proved here.

Table 4.8 The control quality criteria S_u and S_y for predictive control, CSTR

	S_u[-]	S_y[-]
$\lambda_u = 0.05$	1865.00	204.71
λ_u = 0.5	**507.19**	**338.95**
$\lambda_u = 2$	160.12	675.33

THE BEST RESULTS OF EACH CONTROL STRATEGY

All simulation studies were done with the same reference signal for all control strategies presented above, which means that the results are comparable. They are shown

in Figure 4.25 and Table 4.9. These results clearly show that the best result is obtained for the predictive control, although the difference among all strategies is not large.

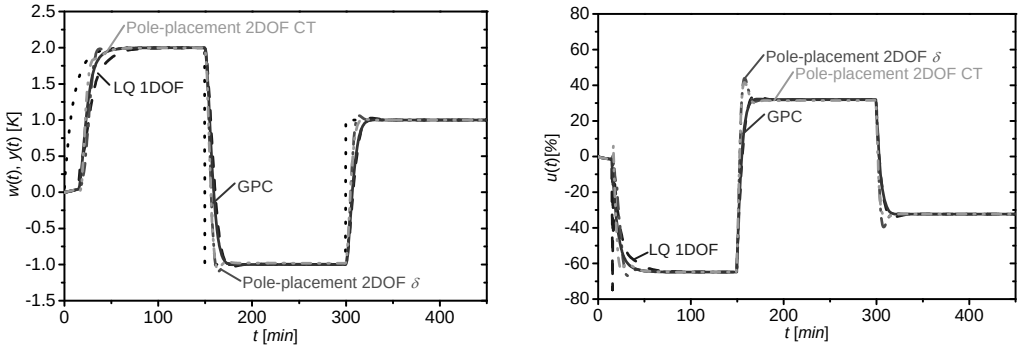


Figure 4.25 The best results of each control strategies, CSTR

Table 4.9 The control quality criteria S_u and S_y for the best results, CSTR

	S_u[-]	S_y[-]
Pole-placement 1DOF, δ-ELM, $\alpha_i = 0.4$	62933	198.81
Pole-placement 2DOF, δ-ELM, $\alpha_i = 0.4$	1059	314.62
LQ 1DOF, $\phi_{LQ} = 0.05$	20824	433.90
LQ 2DOF, $\phi_{LQ} = 0.05$	17260	628.1
Pole-placement 1DOF, CT-ELM, $\alpha_i = 0.4$	25570	93.01
Pole-placement 2DOF, CT-ELM, $\alpha_i = 0.4$	1755	172.86
Predictive control, $\lambda_u = 0.5$	507	338.95

The results presented in the table and the figure above have shown the best results for the predictive control from the output variable and input variable point of view too. The adaptive control with pole-placement method, 2DOF control configuration and CT ELM can be stated as the second best method and the third is in this adaptive control with pole-placement method, 2DOF control configuration and δ-ELM.

4.2 Plug-Flow Reactor (PFR)

The second simulation model is tubular chemical reactor with the ideal plug-flow tubular chemical reaction with a simple exothermic consecutive reaction $A \rightarrow B \rightarrow C$ in the liquid phase and with cooling in the jacket [19]. These types of reactors are called Plug-Flow Reactors (PFR) [4].

4.2.1 Description of the Model

The mathematical description of all quantities and relations among them is very complex and we need some simplifications again. We neglect heat losses and conduction along the metal wall of the pipes, but 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* (black solid line) and *counter-current cooling* (red dashed line). The differences between them are displayed in Figure 4.26 and they will be investigated in static and dynamic analyses.

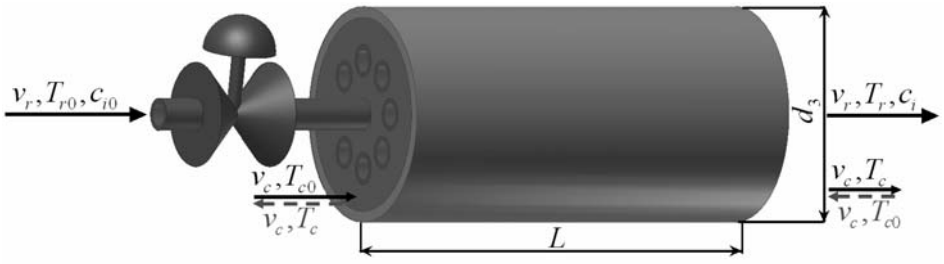


Figure 4.26 PFR with co-current and counter-current cooling in the jacket – the main pipe

The jacket has diameter d_3 and outer diameter of each pipe is d_2, while the inner diameter is denoted as d_1 – see Figure 4.27.

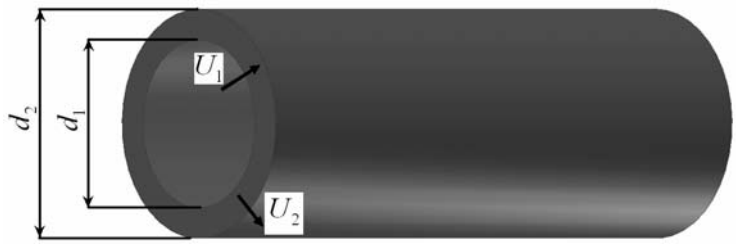


Figure 4.27 PFR – one pipe

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 five Partial Differential Equations (PDE):

$$\begin{aligned}
&\frac{\partial c_A}{\partial t} + v_r \cdot \frac{\partial c_A}{\partial z} = -k_1 \cdot c_A \\
&\frac{\partial c_B}{\partial t} + v_r \cdot \frac{\partial c_B}{\partial z} = k_1 \cdot c_A - k_2 \cdot c_B \\
&\frac{\partial T_r}{\partial t} + v_r \cdot \frac{\partial T_r}{\partial z} = \frac{h_r}{\rho_r \cdot c_{pr}} - \frac{4 \cdot U_1}{d_1 \cdot \rho_r \cdot c_{pr}} \cdot \left(T_r - T_w\right) \\
&\frac{\partial T_w}{\partial t} = \frac{4}{\left(d_2^2 - d_1^2\right) \cdot \rho_w \cdot c_{pw}} \cdot \left[d_1 \cdot U_1 \cdot \left(T_r - T_w\right) + d_2 \cdot U_2 \cdot \left(T_c - T_w\right)\right]
\end{aligned} \tag{4.39}$$

The last PDE for co-current cooling is

$$\frac{\partial T_c}{\partial t} + v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2}{\left(d_3^2 - n_1 \cdot d_2^2\right) \cdot \rho_c \cdot c_{pc}} \left(T_w - T_c\right) \tag{4.40}$$

and for counter-current cooling is this equation (opposite flow of the cooling medium) denoted as

$$\frac{\partial T_c}{\partial t} - v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2}{\left(d_3^2 - n_1 \cdot d_2^2\right) \cdot \rho_c \cdot c_{pc}} \left(T_w - T_c\right) \tag{4.41}$$

where T is the temperature, d represents diameters, ρ are densities, c_p means specific heat capacities, U stands for the heat transfer coefficients, m 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, respectively, as

$$v_r = \frac{q_r}{f_r}; \quad v_c = \frac{q_c}{f_c} \tag{4.42}$$

where q are flow rates and f are constants

$$f_r = n_1 \cdot \frac{\pi \cdot d_1^2}{4}; \quad f_c = \frac{\pi}{4}\left(d_3^2 - n_1 \cdot d_2^2\right) \tag{4.43}$$

The reaction velocities, k_i, in equations (4.39) and (4.41) are nonlinear functions of temperature computed via the Arrhenius law

$$k_j = k_{oj} \cdot \exp\left(-\frac{E_j}{R \cdot T_r}\right), \text{for } j = 1,2 \tag{4.44}$$

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

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B \tag{4.45}$$

and h_j is used for reaction enthalpies.

The mathematical model given in Equations (4.39), (4.40) and (4.41) together with equations (4.44) and (4.45) shows that this plant is a *nonlinear system with continuously distributed parameters* [8]. Strong nonlinearity can be found in Equation (4.44), 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.

In this case 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, input and state variables

Fixed parameters of PFR are displayed in Table 4.10 [19].

Table 4.10 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	$\rho_w = 7800\ kg.m^3$
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	$k_{10} = 5.61\times10^{16}\ s^{-1}$
Pre-exponential factor for reaction 2	$k_{20} = 1.128\times10^{16}\ s^{-1}$
Activation energy of reaction 1 to R	$E_1/R = 13477\ K$
Activation energy of reaction 2 to R	$E_2/R = 15290\ K$
Enthalpy of reaction 1	$h_1 = 5.8\times10^4\ kJ.kmol^{-1}$
Enthalpy of reaction 2	$h_2 = 1.8\times10^4\ kJ.kmol^{-1}$
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 $T_c(z,t)$.

The choice of the input variables is theoretically quite wide – for example all changes of boundary conditions $c_{A0}(t)$, $c_{B0}(t)$, $T_{r0}(t)$, $T_{c0}(t)$ or $T_{cL}(t)$. However, in our case volumetric flow rates q_r and q_c were chosen as input variables because of the practical view again because thez can be easily controlled.

4.2.2 Steady-state Analysis

The difference between the systems with distributed parameters (PFR) and with lumped parameters (CSTR) is that the former takes into account two derivatives – with respect to time and with respect to axial variable. Steady-state analysis means, as in the previous case, solving of the set of PDE (4.39) for time $t \rightarrow \infty$, which means that all derivatives with respect to time are equal to zero. But there are still derivatives with respect to axial variable in the set (4.39) and (4.40).

These derivatives can be replaced from the mathematical point of view by the first back differences

$$\left.\frac{dx}{dz}\right|_{z=z_i} \approx \frac{x(i)-x(i-1)}{h_z}, \text{for } i=1,2,\ldots n \tag{4.46}$$

where x is a general variable, h_z is an optional size of the step in axial direction. The defined input boundary conditions, x_0, for $i = 1$ are equal to boundary conditions $x(0)$. If the reactor is divided into N_z equivalent parts, the discretization step is

$$h_z = \frac{L}{N_z} \tag{4.47}$$

where L denotes the length of the reactor.

Equation (4.46) is valid only for the set of equations (4.39) and (4.40). The system with counter-current cooling which differs only in Equation (4.41) has the boundary condition defined for $z = L$ because of the counter-current cooling in the reactor's jacket. Therefore, the first forward difference must be used

$$\left.\frac{dx}{dz}\right|_{z=z_j} \approx \frac{x(j+1)-x(j)}{h_z}, \text{ for } j = n,\ n\text{-}1,\ldots 0 \tag{4.48}$$

The set of PDE (4.39) is then transformed to a set of nonlinear equations

$$\begin{aligned}
c_A(i) &= \frac{v_r}{v_r + h_z \cdot k_1(i)} \cdot c_A(i-1) \\
c_B(i) &= \frac{h_z}{v_r + h_z \cdot k_2(i)} \cdot \left[k_1(i) \cdot c_A(i) + b_0 \cdot c_B(i-1)\right] \\
T_r(i) &= \frac{d_1 \cdot h_z \cdot Q_r(i) + v_r \cdot d_1 \cdot \rho_r \cdot c_{pr} \cdot T_r(i-1) + 4 \cdot \alpha_1 \cdot h_z \cdot T_w(i)}{v_r \cdot d_1 \cdot \rho_r \cdot c_{pr} + 4 \cdot \alpha_1 \cdot h_z} \\
T_w(i) &= \frac{d_1 \cdot \alpha_1 \cdot T_r(i) + d_2 \cdot \alpha_2 \cdot T_c(i)}{d_1 \cdot \alpha_1 + d_2 \cdot \alpha_2}
\end{aligned} \tag{4.49}$$

and the PDE (4.40) for co-current cooling is

$$T_c(i) = \frac{4 \cdot n_1 \cdot d_2 \cdot \alpha_2 \cdot h_z \cdot T_w(i) + v_c\left(d_3^2 - n_1 \cdot d_2^2\right)\rho_c \cdot c_{pc} \cdot T_c(i-1)}{4 \cdot n_1 \cdot d_2 \cdot \alpha_2 \cdot h_z + v_c\left(d_3^2 - n_1 \cdot d_2^2\right)\rho_c \cdot c_{pc}} \tag{4.50}$$

while for counter-current cooling from the equation (4.41) the cooling temperature, according to first forward difference (4.48), is

$$T_c(j) = \frac{4 \cdot n_1 \cdot d_2 \cdot \alpha_2 \cdot h_z \cdot T_w(j) + v_c\left(d_3^2 - n_1 \cdot d_2^2\right)\rho_c \cdot c_{pc} \cdot T_c(j+1)}{4 \cdot n_1 \cdot d_2 \cdot \alpha_2 \cdot h_z + v_c\left(d_3^2 - n_1 \cdot d_2^2\right)\rho_c \cdot c_{pc}} \tag{4.51}$$

The computation of reaction rates k_1, k_2 and reaction heat Q_r from the equations (4.44) and (4.45) must be discretized too, i.e.

$$\begin{aligned}
k_j(i) &= k_{oj} \cdot \exp\left(-\frac{E_j}{R \cdot T_r(i)}\right), \text{for } j = 1,2 \\
Q_r(i) &= h_1 \cdot k_1(i) \cdot c_A(i) + h_2 \cdot k_2(i) \cdot c_B(i)
\end{aligned} \tag{4.52}$$

The set of nonlinear equations (4.49), (4.50) and (4.51) must be solved with the use of iterative methods (Chapter 3.1.3) because the reactive heat, Q_r, is a nonlinear function of the reactive temperature, T_r, as can be seen in (4.52). The second reason for the use of the iterative method is that the boundary condition for the cooling liquid in Equation (4.51) is defined for axial variable $z = L$.

In the iterative computation two cycles were used. The outer cycle is iterative and the inner cycle computes steady-state values in every axial span along the length of the reactor. The iterative computation is stopped when the sum of the differences between the mean temperature of the reactant and the cooling liquid in the actual step and in previous step is lower than accuracy ε, i.e.

$$\left|\overline{T}_r\left(st\right)-\overline{T}_r\left(st-1\right)\right|+\left|\overline{T}_c\left(st\right)-\overline{T}_c\left(st-1\right)\right|<\varepsilon \quad \text{for } st = 1, 2,\ldots, N_z \tag{4.53}$$

for $\varepsilon = 1\cdot10^{-3}$, st indicates the iterative step, and the mean temperatures are computed via

$$\overline{T}_r\left(st\right)=\frac{1}{N_z}\cdot\sum_{i=1}^{N_z}T_r\left(i\right);\quad \overline{T}_c\left(st\right)=\frac{1}{N_z}\cdot\sum_{i=1}^{N_z}T_c\left(i\right) \tag{4.54}$$

The first analysis was done for different volumetric flow rates of the cooling liquid which is used in variable v_c in equations (4.49) – (4.51), see Equation (4.42). The steady-state behaviour was examined for the range $q_c^s = \langle 0.1;\ 0.35\rangle$ $[m^3.s^{-1}]$ (x-axis). Only the results for the product's concentration, c_B^s, and the reactant's temperature, T_r^s, are shown here, because of the length of the thesis. In the following 3D graphs the steady-state values are displayed on the z-axis, and the length of the reactor is on the y-axis.

Figure 4.28 and Figure 4.29 display the results for the co- and counter-current cooling in the jacket; it can be clearly seen that counter-current cooling results in high nonlinearity whereas in co-current cooling the variables are much more linear.

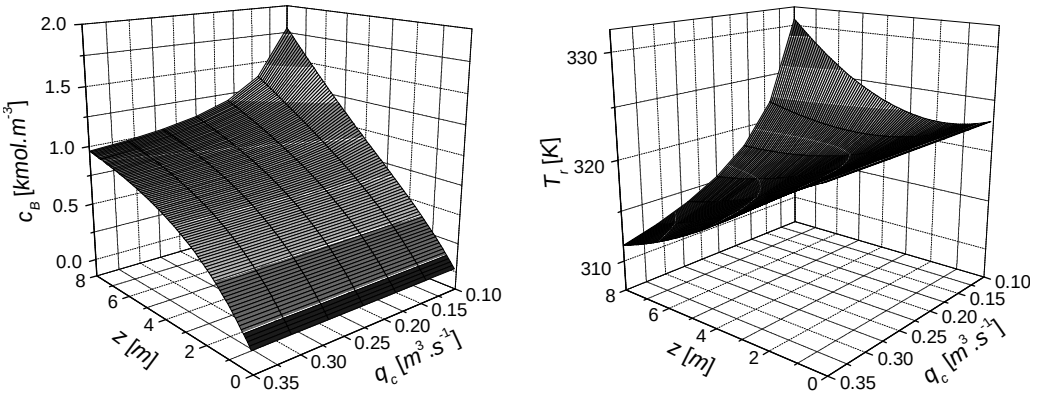


Figure 4.28 Steady-state values of c_B^s and T_r^s for different volumetric flow rates of the cooling liquid, q_c, co-current cooling, PFR

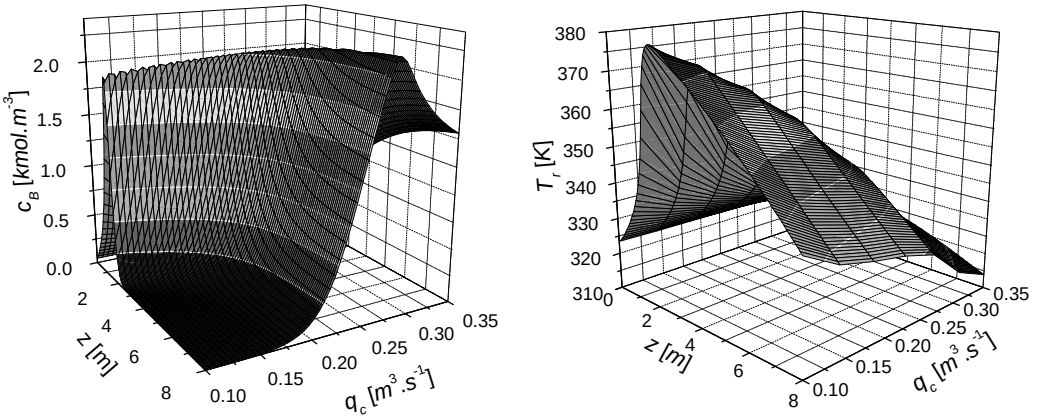


Figure 4.29 Steady-state values of c_B^s and T_r^s for different volumetric flow rates of the cooling liquid, q_c, counter-current cooling, PFR

The second steady-state analysis was done for the same variables but for different values of the volumetric flow rate of the reactant q_r^s = <0.1; 0.35> [$m^3.s^{-1}$]. The results are shown in Figure 4.30 and Figure 4.31. The graphs indicate similar behaviour as in the previous analysis – counter-current cooling is much more non-linear.

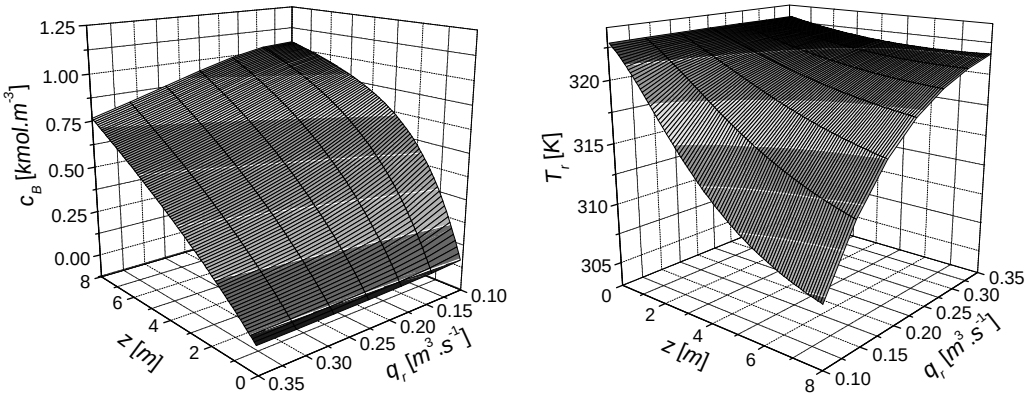


Figure 4.30 Steady-state values of c_B^s and T_r^s for different volumetric flow rated of the reactant, q_r, co-current cooling, PFR

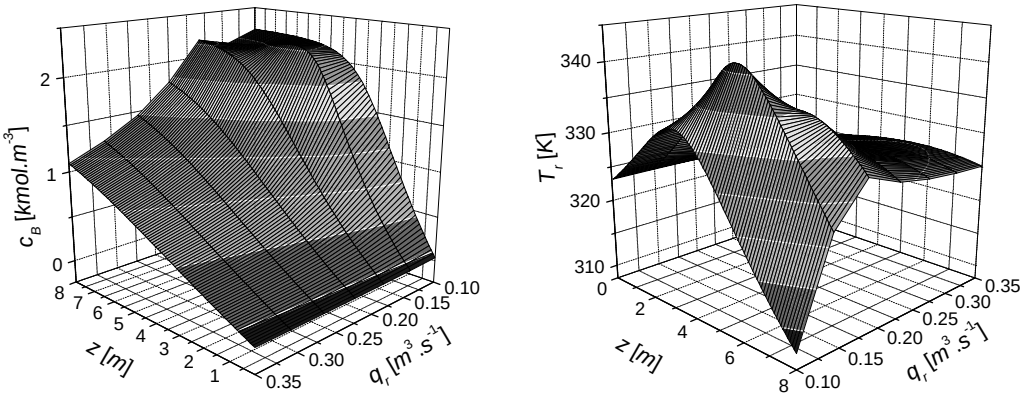


Figure 4.31 Steady-state values of c_B^s and T_r^s for different volumetric flow rates of the reactant, q_r, counter-current cooling, PFR

The steady-state analysis results in the working point similarly as for the CSTR. The optimal working point in this case is defined by the volumetric flow rate of the reactant $q_r^s = 0.150\ m^3.s^{-1}$ and the volumetric flow rate of the coolant $q_c^s = 0.275\ m^3.s^{-1}$. These variables are later used for dynamic analysis and simulation of the control.

4.2.3 Dynamic Analysis

Dynamic analysis is the next step after the steady-state analysis. It examines the behaviour after the step change of one of the input variables. Because the set of PDE (4.39), (4.40) has derivatives with the respect to axial variable z, the discretization described by equations (4.46) and (4.48) must be used. The set of PDE is then transformed to a set of ODE:

$$\begin{aligned}
\frac{dc_A(i)}{dt} &= -\left[\frac{v_r}{h_z} + k_1(i)\right]\cdot c_A(i) + \frac{v_r}{h_z}\cdot c_A(i-1) \\
\frac{dc_B(i)}{dt} &= -\left[\frac{v_r}{h_z} + k_2(i)\right]\cdot c_B(i) + \frac{v_r}{h_z}\cdot c_B(i-1) + k_1(i)\cdot c_A(i) \\
\frac{dT_r(i)}{dt} &= -\left[\frac{v_r}{h_z} + \frac{4\cdot\alpha_1}{d_1\cdot\rho_r\cdot c_{pr}}\right]\cdot T_r(i) + \frac{v_r}{h_z}\cdot T_r(i-1) + \frac{Q_r(i)}{\rho_r\cdot c_{pr}} + \frac{4\cdot\alpha_1}{d_1\cdot\rho_r\cdot c_{pr}}\cdot T_w(i) \\
\frac{dT_w(i)}{dt} &= -\left[\frac{4\cdot(d_1\cdot\alpha_1 + d_2\cdot\alpha_2)}{(d_2^2 - d_1^2)\cdot\rho_w\cdot c_{pw}}\right]\cdot T_w(i) + \frac{4\cdot d_1\cdot\alpha_1}{(d_2^2 - d_1^2)\cdot\rho_w\cdot c_{pw}}\cdot T_r(i) + \frac{4\cdot d_2\cdot\alpha_2}{(d_2^2 - d_1^2)\cdot\rho_w\cdot c_{pw}}\cdot T_c(i)
\end{aligned} \tag{4.55}$$

For the co-current cooling the last equation for the cooling temperature, T_c, has the following form

$$\frac{dT_c(i)}{dt} = -\left[\frac{v_c}{h_z} + \frac{4\cdot n_1\cdot d_2\cdot\alpha_2}{(d_3^2 - n_1\cdot d_2^2)\cdot\rho_c\cdot c_{pc}}\right]\cdot T_c(i) + \frac{v_c}{h_z}\cdot T_c(i-1) + \frac{4\cdot n_1\cdot d_2\cdot\alpha_2}{(d_3^2 - n_1\cdot d_2^2)\cdot\rho_c\cdot c_{pc}}\cdot T_w(i) \tag{4.56}$$

whereas this relation for the counter-current cooling is

$$\frac{dT_c(j)}{dt} = -\left[\frac{v_c}{h_z} + \frac{4\cdot n_1\cdot d_2\cdot\alpha_2}{(d_3^2 - n_1\cdot d_2^2)\cdot\rho_c\cdot c_{pc}}\right]\cdot T_c(j) + \frac{v_c}{h_z}\cdot T_c(j+1) + \frac{4\cdot n_1\cdot d_2\cdot\alpha_2}{(d_3^2 - n_1\cdot d_2^2)\cdot\rho_c\cdot c_{pc}}\cdot T_w(j) \tag{4.57}$$

Again, the computation runs in two cycles. The outer cycle solves numerically the set of ODE (4.55), (4.56) and (4.57) with the use of Runge-Kutta's standard method described in Chapter 3.1.4. The inner cycle divides the reactor into N_z equivalent pieces and computes dynamics in each part.

Stready-state values from the previous part were used as input variables to the dynamic analysis, as shown in previous case for CSTR and the standard Runge Kutta's method of fourth degree was used for solving this set of ODE [6]. Two dynamic analyses were done – the first for four step changes ±20% and ±10% of the volumetric flow rate of the cooling liquid, Δq_c^s, and the volumetric flow rate of the reactant, Δq_r^s, is –0.055 (–20%), –0.0275 (–10%), 0.0275 (10%), 0.055 (20%) $m^3.s^{-1}$ for Δq_c^s and –0.03 (–20%), –0.015 (–10%), 0.015 (10%), 0.03 (20%) $m^3.s^{-1}$ for Δq_r^s.

These input variables should be mathematically described as

$$u(t)=\frac{q_c(t)-q_c^s}{q_c^s}\cdot 100;\; u(t)=\frac{q_r(t)-q_r^s}{q_r^s}\cdot 100 \quad [\%] \tag{4.58}$$

Output variables y_1 and y_2 in the following figures illustrate the difference between the actual values of the product's concentration c_B, the reactive temperature, T_r, at the end of the reactor ($z = L$) and their steady-state values c_B^s and T_r^s.

$$y_1(t)=c_B(t,L)-c_B^s(L)\left[kmol.m^{-3}\right];\quad y_2(t)=T_r(t,L)-T_r^s(L)\left[K\right] \tag{4.59}$$

Simulation analyses were done again for co-current and counter-current cooling.

Figure 4.32 and Figure 4.33 show dynamic responses for various step changes of input volumetric flow rates q_c^s and q_r^s with co-current cooling in the jacket.

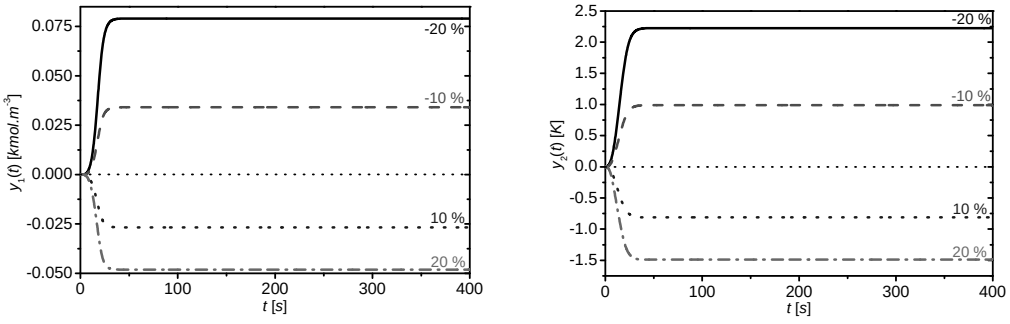


Figure 4.32 Output responses of outputs $y_1(c_B)$ and $y_2(T_r)$ for various step changes of the volumetric flow rate of cooling liquid, Δq_c^s, co-current cooling, PFR

These output variables can be described by the second order transfer function, except for y_1 which represents the output concentration, c_B, for the step change of the volumetric flow rate on the input. This variable has a very nonlinear course and it can mean substantial problems in control.

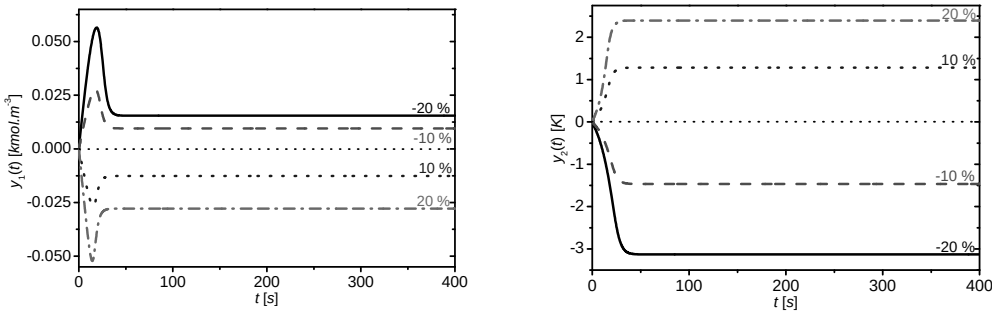


Figure 4.33 Output responses of outputs $y_1(c_B)$ and $y_2(T_r)$ for various step changes of the volumetric flow rate of the reactant, Δq_r^s, co-current cooling, PFR

Dynamic analysis for the counter-current cooling presented in Figure 4.34 and Figure 4.35 has all negative properties from the control point of view, such as non-minimum phase behaviour (output y_1) and time delay.

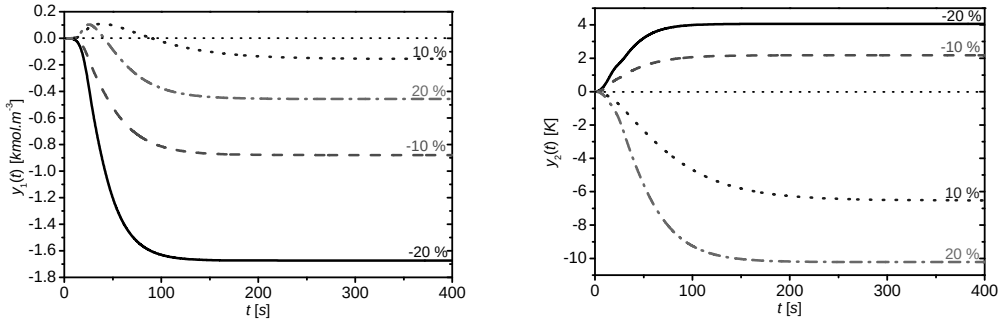


Figure 4.34 Output responses of outputs $y_1(c_B)$ and $y_2(T_r)$ for various step changes of the volumetric flow rate of the cooling liquid, Δq_c^s, counter-current cooling, PFR

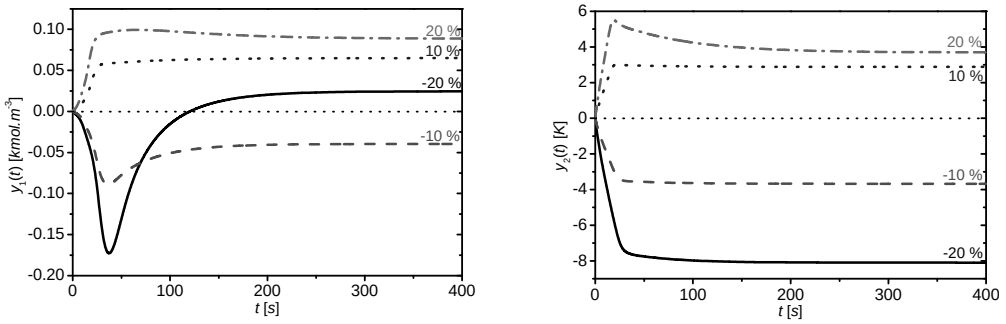


Figure 4.35 Output responses of outputs $y_1(c_B)$ and $y_2(T_r)$ for various step changes of the volumetric flow rate of the reactant, Δq_r^s, counter-current cooling, PFR

The last dynamic analysis compares co-current and counter-current cooling for the same step changes of the input variables. Although the properties of the counter-current system are not very good for control, it is often used because this type of cooling has a better cooling effect. This can bee clearly seen in Figure 4.36 and Figure 4.37 – with the same step change of volumetric flow rates Δq_r^s and Δq_c^s, the stable value of product's temperature T_r (output y_2) in counter-current is doubled compared to co-current configuration. Output concentration y_1 has an interesting course too – non-minimum phase behaviour and the changing sign of gain.

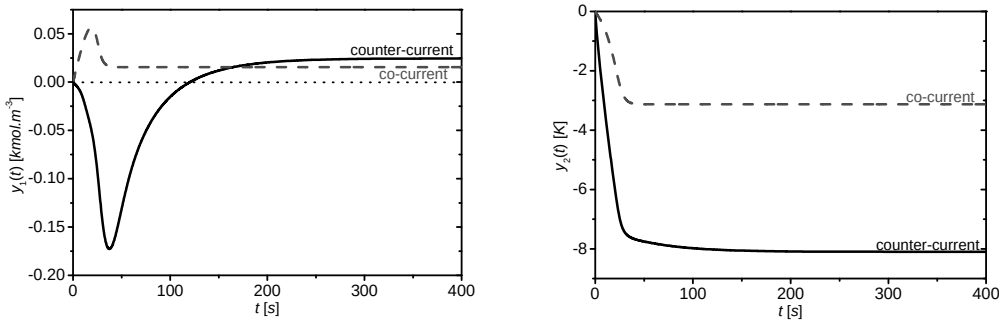


Figure 4.36 Comparison of co-current and counter-current cooling for outputs $y_1(c_B)$ and $y_2(T_r)$, step change of the volumetric flow rate of the reactant Δq_r^s = -20%, PFR

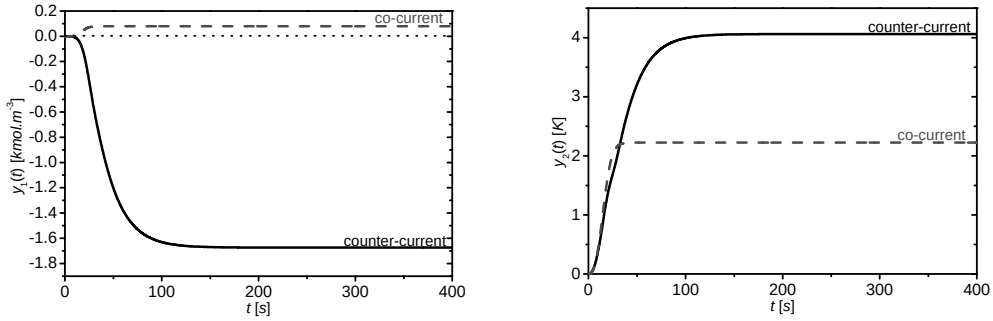


Figure 4.37 Comparison of co-current and counter-current cooling for outputs $y_1(c_B)$ and $y_2(T_r)$, step change of the volumetric flow rate of the cooling Δq_c^s = -20%, PFR

4.2.4 Simulation of Control

This chapter will present only some of the simulation results of the control of the PFR because of the space. The goal is to show that control strategies used for the control of the CSTR in the previous case can be implemented to other types of chemical reactors.

The change of the volumetric flow rate of the reactant, q_c^s, was used as a control (input) variable and the output temperature of the reactant, T_r, related to its steady-state value was used as a controlled (output) variable

$$u(t) = \frac{q_c(t) - q_c^s}{q_c^s} \cdot 100\,[\%];\; y(t) = T_r(t) - T_r^s\,[K] \tag{4.60}$$

The same second-order transfer function with relative order one, similar to the previous case

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0} \tag{4.61}$$

was used as ELM according to the dynamic analysis from the previous chapter and the RLS method with changing exponential forgetting was used for parameter estimation, the same as for CSTR model in Chapter 4.1.4.

The working point and initial values for identification for the simulation of the control are shown in Table 4.11.

Table 4.11 Working point and parameters of the identification used for the control, PFR

Name of the parameter	Symbol and value of the parameter
Input concentration of compound A Input temperature of the reactant Input temperature of the coolant Input volumetric flow rate of the reactant Input volumetric flow rate of the coolant	$c_{A0} = 2.85\ kmol.m^{-3}$ $T_{r0} = 323\ K$ $T_{c0} = 293\ K$ $q_r^s = 0.15\ m^3.s^{-1}$ $q_c^s = 0.275\ m^3.s^{-1}$
Starting vector of parameters	$\boldsymbol{\theta}_\delta(0) = [0.1, 0.1, 0.1, 0.1]^T$
Starting covariance matrix	$\mathbf{P}(0) = \begin{bmatrix} 1\cdot10^6 & 0 & 0 & 0 \\ 0 & 1\cdot10^6 & 0 & 0 \\ 0 & 0 & 1\cdot10^6 & 0 \\ 0 & 0 & 0 & 1\cdot10^6 \end{bmatrix}$

The quality of control was evaluated the quality criteria S_u and S_y described in Equation (4.13).

To be able to compare the results for all control strategies (shown at the end of this chapter), the time of the simulation, T_f, was 6000 s, the sampling period T_v = 1.5 s, the input variable was limited to $u(t)$ = <-80;+80> % of q_c^s and three step changes were done during this time:

$$\begin{aligned} w(t) &= 1\cdot[1-\exp(-0.03\cdot t)]\ K && \text{for } t \in \langle 0;2000\rangle\ s \\ w(t) &= -0.5\ K && \text{for } t \in (2000;4000)\ s \\ w(t) &= 2\ K && \text{for } t \in \langle 4000;6000\rangle\ s \end{aligned} \tag{4.62}$$

ADAPTIVE CONTROL WITH POLE-ASSIGNMENT METHOD

As written above, the same ELM (4.12) was used as the representation of a nonlinear system which means that the controller has the same structure and the parameters of the controller are computed similarly as for CSTR in the previous case.

The transfer function of the controller with 1DOF control configuration is given by Equation (4.18), and parameters of polynomials $q(s)$ and $\tilde{p}(s)$ are computed from the Diophantine equation(4.16). Stable polynomial $d(s)$ is designed via pole-placement method connected with the spectral factorization, i.e. $d(s) = n(s) \cdot m(s)$. This method is described in the previous case.

The ELM is from the range of δ-models, which means that the vector of the parameters, $\boldsymbol{\theta}_\delta$, and the data vector, $\boldsymbol{\varphi}_\delta$, are

$$\begin{aligned} \boldsymbol{\theta}_\delta(k) &= \left[a_1', a_0', b_1', b_0'\right]^T \\ \boldsymbol{\varphi}_\delta(k-1) &= \left[-y_\delta(k-1), -y_\delta(k-2), u_\delta(k-1), u_\delta(k-2)\right]^T \end{aligned} \tag{4.63}$$

The vector of parameters, $\boldsymbol{\theta}_\delta$, is estimated recursively during control with the help of any RLS method with the initial values from Table 4.2.

The simulation study is done for different values of parameter α_i = 0.01, 0.02 and 0.03. The results presented in Figure 4.38 show that the proposed adaptive controller has a problem with control only at the very beginning of control, where it does not have enough information about the system. Once the parameters are adapted sufficiently, the control response has good results. The increasing value of parameter α_i affects mainly the speed of response, the overshoots are comparably high. Although the input variable, $u(t)$, for the highest value α_i = 0.03 has not an ideal course (with a lot of shocking changes), the controller with this setting has the best course of the output variable. The values of criteria S_u and S_y are displayed in the Table 4.12.

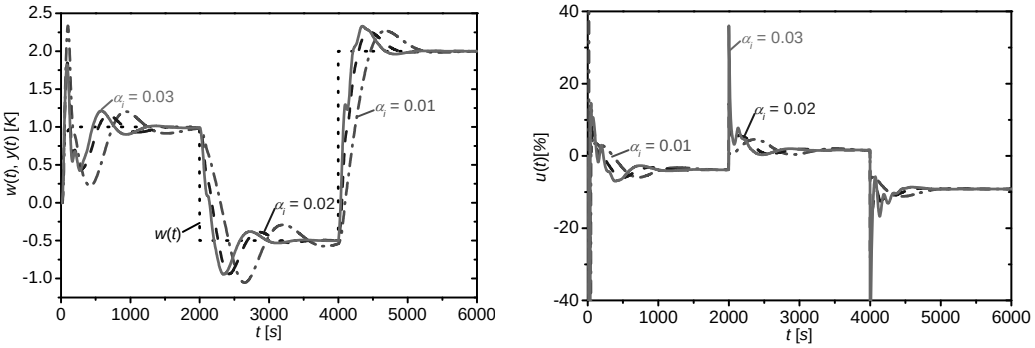


Figure 4.38 The course of $y(t)$, $w(t)$ and $u(t)$ for different position of the parameter α_i = 0.01, 0.02 and 0.03, 1DOF, pole-placement method, δ-ELM, PFR

The graphs in Figure 4.39 show the results of the recursive identification during simulation. It can be clearly seen that the used identification has no substantial problem with the adaptation, except at the beginning of the control. The course of identified parameter b'_0 shows that this parameter is very small and is not changing during the control.

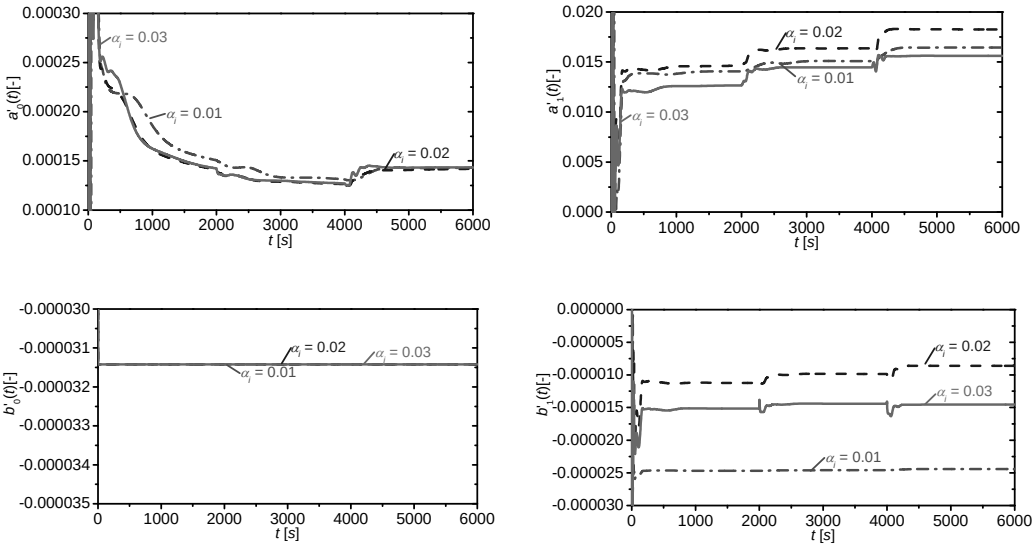


Figure 4.39 The course of identified parameters a'_0, a'_1, b'_0 and b'_1 during the control, 1DOF, pole-placement method, δ-ELM, PFR

Table 4.12 The control quality criteria S_u, S_y for pole-placement method, δ-ELM, PFR

	S_u[-]	S_y[-]
$\alpha_i = 0.01$	70789.83	1141.70
$\alpha_i = 0.02$	7555.19	568.15
$\alpha_i = 0.03$	**13861.81**	**425.01**

The effect of disturbances is displayed in Figure 4.40. The simulation time in this case is 10 000 *s* and the value of criterion α_i is 0.008. Three disturbances are injected to the system:

- $v_1(t)$ = +1.5% step change of the input concentration c_{A0} for time $t \in \langle 3000;10000 \rangle s$
- $v_2(t)$ = 0.25 *K* step change of the input temperature T_{r0} for time $t \in \langle 5000;10000 \rangle s$
- $v_3(t)$ = -0.2 *K* step change of the output temperature T_r for time $t \in \langle 7000;10000 \rangle s$

The course of the output variable shows that the proposed controller has no problem to deal with these three disturbances – see Figure 4.40. The values of control quality criteria are S_u = 30382.23 and S_y = 284.03.

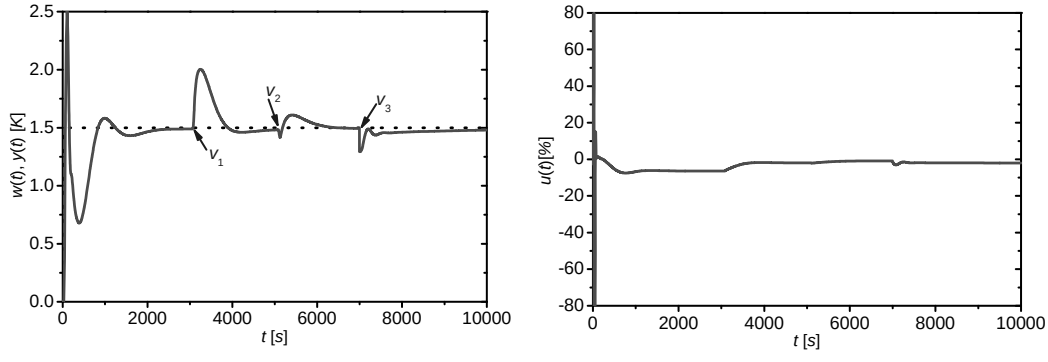


Figure 4.40 The course of $y(t)$, $w(t)$ and $u(t)$ for three disturbances, α_i = 0.008, 1DOF, pole-placement method, δ-ELM, PFR

ADAPTIVE CONTROL WITH LQ APPROACH

The second control analysis was done for the adaptive controller based on LQ approach, similarly to CSTR. The parameters of stable polynomial $d(s)$ on the right side of the Diophantine equation (4.16) are computed by minimizing of the cost function (3.112). The control simulation is done for three different values of weighting factor ϕ_{LQ} = 0.005, 0.01 and 0.02, and the second weighting factor is μ_{LQ} = 1 for all simulations.

The output variable $y(t)$ in Figure 4.41 has similar courses as for adaptive control with pole-placement method presented in the previous chapter. The increasing value of weighting factor ϕ_{LQ} results in bigger overshoots and slower course of the output variable.

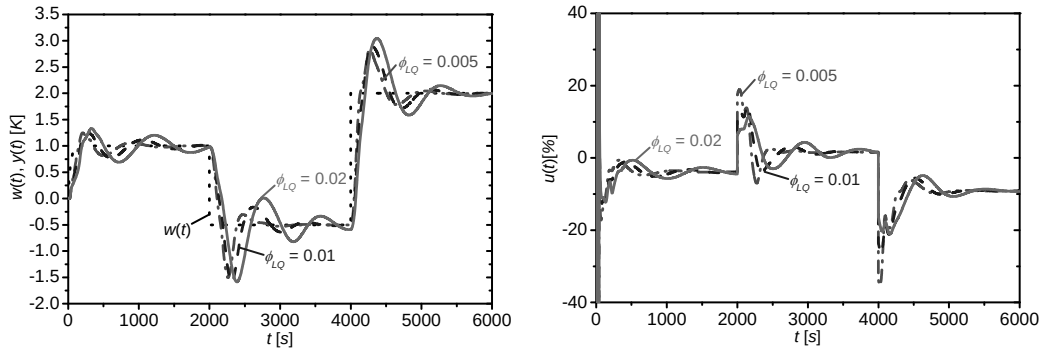


Figure 4.41 The course of $y(t)$, $w(t)$ and $u(t)$ for different weighting factor ϕ_{LQ} = 0.005, 0.01 and 0.02, 1DOF, LQ method, δ-ELM, PFR

The RLS with a changing forgetting factor has no bigger problems with on-line identification of the process – see Figure 4.42.

The values of criteria S_u and S_y shown in Table 4.13 indicate similar control results for all three simulation studies. The best results can be seen for the controller with weighting factor ϕ_{LQ} = 0.005 for both criteria, S_u and S_y.

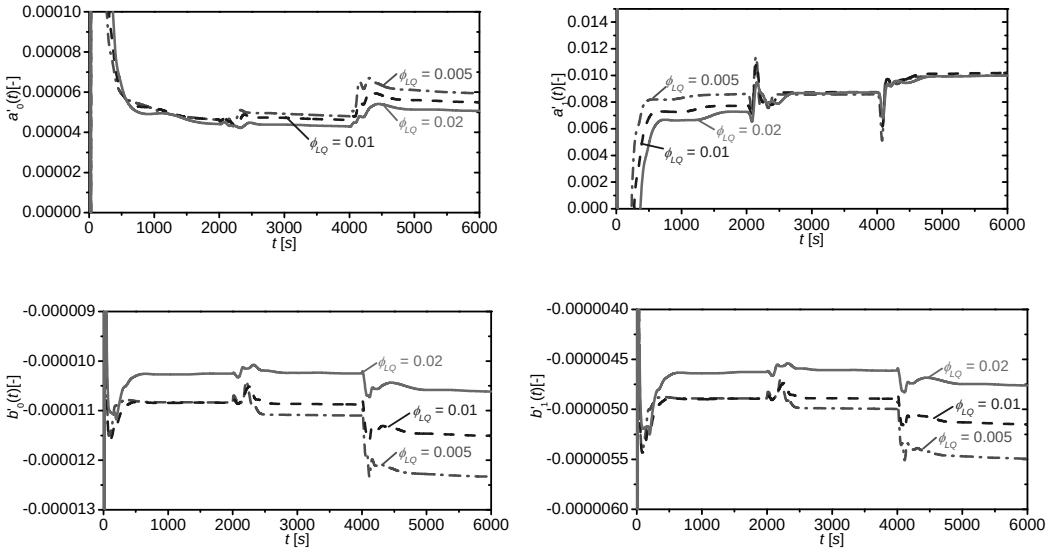


Figure 4.42 The course of identified parameters a'_0, a'_1, b'_0 and b'_1 during the control, 1DOF, LQ method, δ-ELM, PFR

Table 4.13 The control quality criteria S_u, S_y for LQ method, δ-ELM, PFR

	S_u[-]	S_y[-]
ϕ_{LQ} = 0.005	**118631**	**405.03**
ϕ_{LQ} = 0.01	120298	504.75
ϕ_{LQ} = 0.02	119321	646.08

PREDICTIVE CONTROL

Similar generalized predictive control as for CSTR was used in the last control simulation study. The sampling period in this case was T_v = 0.9 *s*, the parameters of the prediction horizon N_1 = 0, N_2 = 50 and N_u = 10 steps. Weighting factors were again constant during the control. The first factor, δ_u = 1, is the same for all and the second differs for particular simulation studies – λ_u = 0.5, 1 and 2.

The discrete transfer function, $G(z)$, obtained from the preidentification has form

$$G\left(z^{-1}\right)=\frac{9.2314\cdot10^{-6}z^{-1}-3.1421\cdot10^{-5}z^{-2}}{1-1.9772z^{-1}+0.9773z^{-2}} \tag{4.64}$$

The simulation results presented in Figure 4.43 show that the course of the output variable is quicker for the lower value of parameter λ_u – see the course for $\lambda_u = 0.5$.

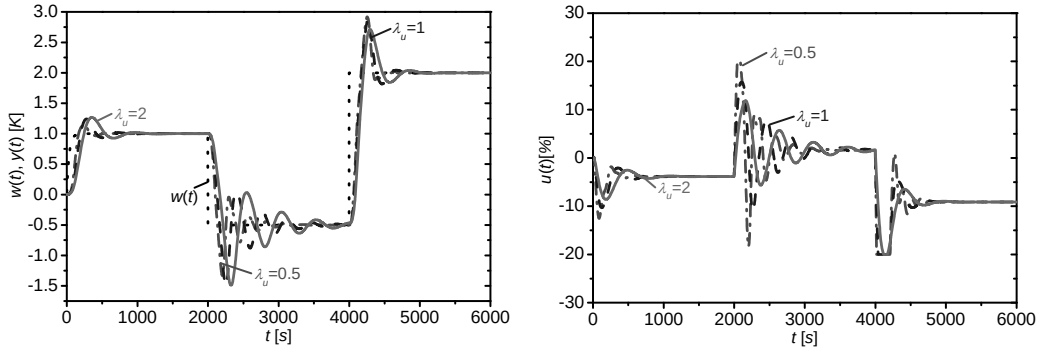


Figure 4.43 The course of $y(t)$, $w(t)$ and $u(t)$ for predictive control and different values of $\lambda_u = 0.5$, 1 and 2, PFR

This contention is supported by the values of quality criteria S_y in Table 4.14, which is the lowest for $\lambda_u = 0.5$. On the other hand, the bigger value of this criterion gives better results from the input variable point of view, which is indicated by the S_u-value in Table 4.14.

Table 4.14 The control quality criteria S_u, S_y for predictive control, PFR

	S_u[-]	S_y[-]
$\lambda_u = 0.5$	**151.80**	**633.81**
$\lambda_u = 1$	51.00	759.63
$\lambda_u = 2$	18.81	980.26

THE BEST RESULTS OF EACH CONTROL STRATEGY

Similarly as for the previous simulation model, the best results from each control strategy are compared in Figure 4.44 and Table 4.15. It can be said that the predictive control approaches to the reference signal in the best way except for the second step change from 1 *K* to -0.5 *K*.

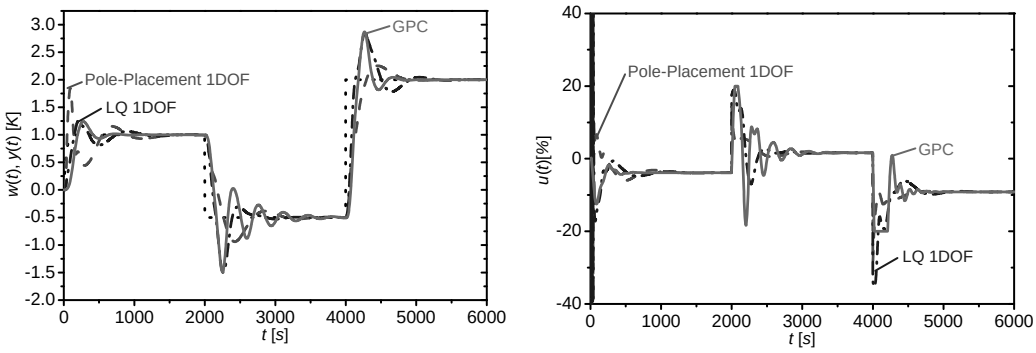


Figure 4.44 The the best results of each control strategy, PFR

Table 4.15 The control quality criteria S_u and S_y for the best results, PFR

	S_u[-]	S_y[-]
Pole-placement 1DOF, δ-ELM, $\alpha_i = 0.03$	13861	425
LQ 1DOF, $\phi_{LQ} = 0.005$	118631	405
Predictive control, $\lambda_u = 0.5$	1251	634

The best results from the criterion S_u and S_y point of view has again predive control, especially if the input variable, $u(t)$, has significant importance. On the other hand, the adaptive controller with LQ approach has the best course of the output variable $y(t)$.

4.3 Real Model of CSTR

The simulation experiments are not fully credible if they are not verified by experiments on a real model. Thus, the proposed controllers from the previous parts were verified on a multifunctional process control teaching system – The Armfield PCT 40 [60]. This device is designed especially for teaching of a wide range of technological and chemical processes, such as temperature control in heat exchangers, flow control, level control in water tanks, pressure control and finally conductivity and pH control in additional PCT 41 and 42 units [61] and [62], which is CSTR. The schematic representation of the model is displayed in Figure 4.45.

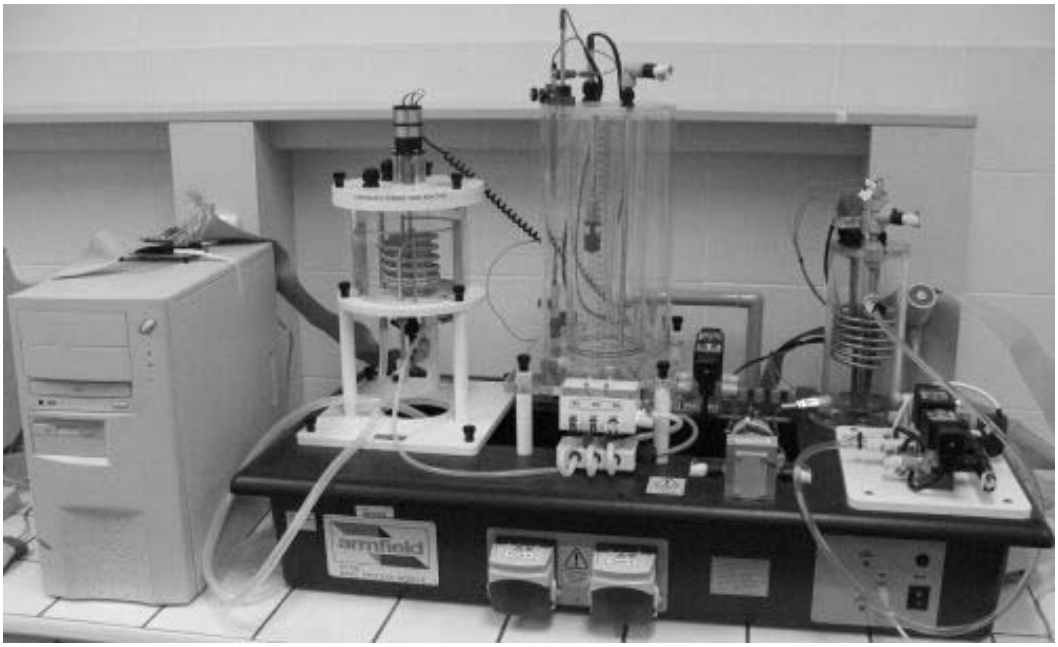


Figure 4.45 Multifunctional Process Control Teaching System PCT40 with additional CSTR (PCT41 and 42)

PCT40 unit consists of two process vessels, several pumps, sensors and connection to the computer. Additional PCT 41 and 42 units represent a chemical reactor with a stirrer inside and a cooling/heating lid.

Figure 4.46 PCT41 and PCT 42 – Process Vessel Accessory (CSTR)

Water can be injected inside the reactor via a normally closed solenoid valve (SOL1) or by a Proportional Solenoid Valve (PSV). The third option how to feed water inside the system is with the use of one of peristaltic pumps, A or B, and the second pump could be used for reactant feeding. This option was used in the following studies. Used pumps and solenoids are shown in Figure 4.47.

Figure 4.47 Solenoid valve SOL1, proportional solenoid valve PSV and peristaltic pumps A, B

The technological parameters of the reactor are shown in the following table.

Table 4.16 Technological parameters of CSTR

Parameter	Range
Vessel diameter	0.153 *m*
Maximum vessel depth	0.108 *m*
Maximum operation volume	2 *l*
Minimum vessel depth	0.054 *m*
Minimum operation volume	1 *l*

Two types of connection are at the disposal (see Figure 4.48). The first connection with Universal Serial Bus (USB) is included in the standard packing. This connection uses special software, ArmSoft, which is also included in the package.

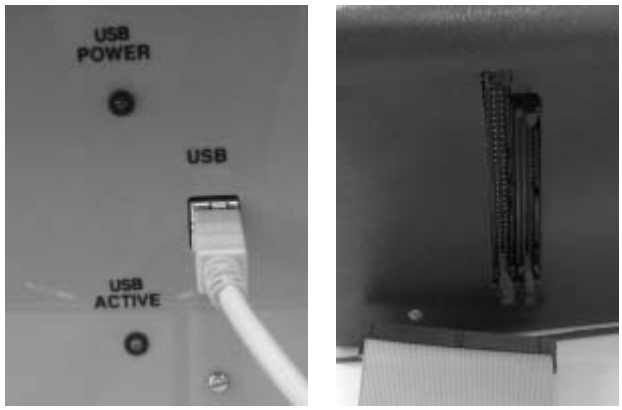


Figure 4.48 USB and 60-way I/O connectors

The view of the main window is in Figure 4.49. The system includes a lot of pre-defined exercises or possibilities to create one's own project work. The computer can communicate with all sensors in real-time via USB cable and the software has implemented basic PID controller with adjustable parameters.

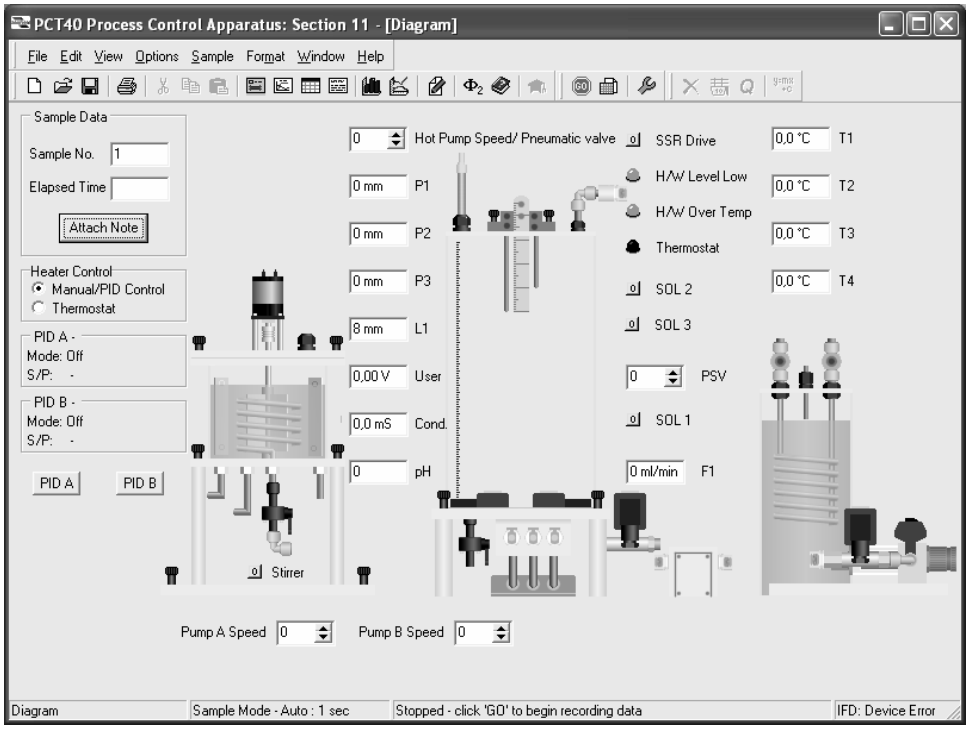


Figure 4.49 ArmSoft simulation system

A disadvantage of this system is that there is no possibility to implement other control strategies programmed in Matlab, C++ etc. This disadvantage can be overcome with the second type of connection via a 60-way I/O connector or 50-way I/O connector to a technological PCI cart in the computer. The technological card used in this case is MF624 multifunction I/O card from Humusoft. This card has 8 inputs and 8 outputs, which is sufficient if we operate only one control exercise at a time. The whole system provides 9 inputs and 17 outputs if all exercises work at in the same time. That is why we use two MF624 cards.

The connection to PC via MF624 cards makes all control exercises fully programmable with the use of Matlab's Real-time toolbox and Simulink (Figure 4.50), or from the Matlab's command window.

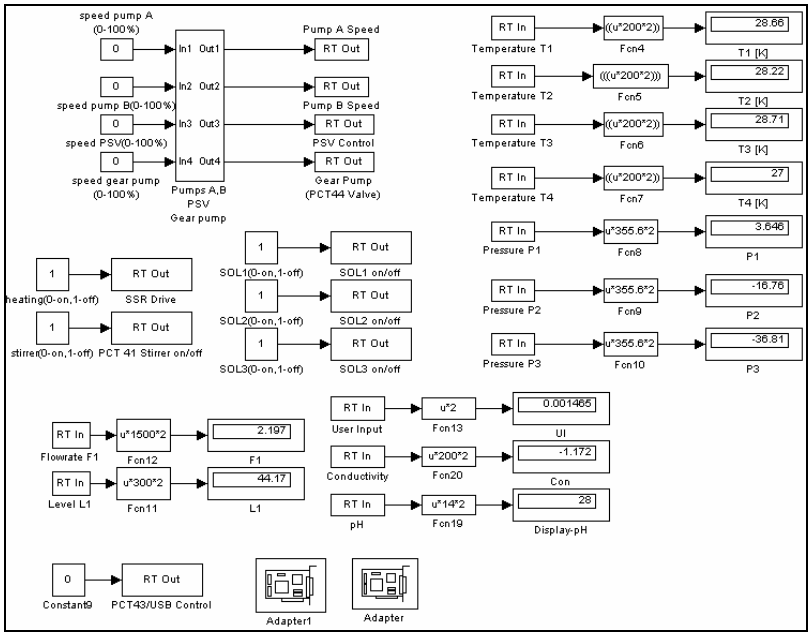


Figure 4.50 Basic Simulink scheme

All measurements and control signals in the work were made from Matlab's command window via commands `rtin` and `rtout`.

4.3.1 Description of the Chemical Process

The producer of PCT40 recommends dilution of potassium bicarbonate ($KHCO_3$) in water. This chemical is non-toxic and the conductivity control could be carried out in safe conditions of temperature and pressure. However, in our case potassium bicarbonate was replaced by ordinary sodium chloride (NaCl). The main reason of this substitution was the cost of experiment – twenty liters of 20% solution of potassium bicarbonate is made from 4.5 *kg* of dry $KHCO_3$, which costs about 1350 Czech crowns, and the same amount of NaCl costs 18 Czech crowns, which is 75 times less than $KHCO_3$. This substitution was made with the agreement of Armfield, the producer of the PCT40.

Thus, the chemical used in the experiments was 5% solution of NaCl, which means that 20 litres of the chemical consists of 1 *kg* dry NaCl solved in 19.5 litres of water. The

conductivity of this solution is about 60 *mS*, which is relatively high and suitable for basic experiments. The conductivity, which will be controlled, changes with the degree of sality.

Other conditions which are common for all measurements are:

- The chemical and water are fed in the reactor by peristaltic pumps viewed in Figure 4.43. Volumetric flow rates of these pumps could be theoretically set in the range 0÷100 %; however, setting lower than 20% results in very small revolutions of the rotor and the produced force is not high enough to transport the fluid from the barrel. The range set into the input recomputed to the volumetric flow rate is shown in Table 4.17.

Table 4.17 Speed of pumps A and B in *%* recomputed to the flow rate in $l.min^{-1}$.

Range set at the input to pumps A and B	Flow rate of pump A[$l.min^{-1}$]	Flow rate of pump B [$l.min^{-1}$]
100%	1.12	1.11
75%	0.80	0.80
50%	0.48	0.51
30%	0.22	0.26

- Although the system could be understood as multi-input (input flow rate of water and 5% salt solution) single-output (conductivity), only flow rate of water was used as a manipulated (input) variable. The flow rate of the chemical for all measurements is set to 30% (0.26 $l.min^{-1}$).
- The overflow inside the reactor is in the minimum position, which means that the volume of the reactor is minimal, i.e. 1 liter. This setting is done because of minimal cost of the experiment.
- The reactor is cleaned and fed with clean water before each experiment to ensure the same starting conditions. It means that at the beginning the conductivity of the bulk chemical is close to zero.

- It is expected that the system belongs to the class of lumped parameters systems which, means that the state variable (in our case the conductivity) depends only on the time variable. This condition is fulfilled with the stirrer switched on during measurements. The stirrer has only two states – on/off and the revolutions are not adjustable.
- Even though the reactor has a heating/cooling coil, this equipment is not used in the experiments.
- The used clean water is ordinary cold water from the standard water distribution.

4.3.2 Static and Dynamic Analyses

The static study displays steady-state values of the conductivity. It can be said that the system has mostly linear behaviour for the input variable u = 30÷70 %, which is represented by the volumetric flow rate of clean water through peristaltic pump A. As can be seen in Figure 4.51, the static behaviour for interval u = 70÷100 % has nonlinear behaviour. The flow rate lower than 30% was not taken into the examination because the revolvations of the pump is too low – see the remarks above.

Dynamic analysis was done for six step changes of volumetric flow rate – Δu = 30%, 40%, 55%, 70%, 85% and 100%. The time of the measurement is 720 *s* (12 *min*) and the sampling period for the values retrieval is T_v = 1 *s*. The results are in Figure 4.51.

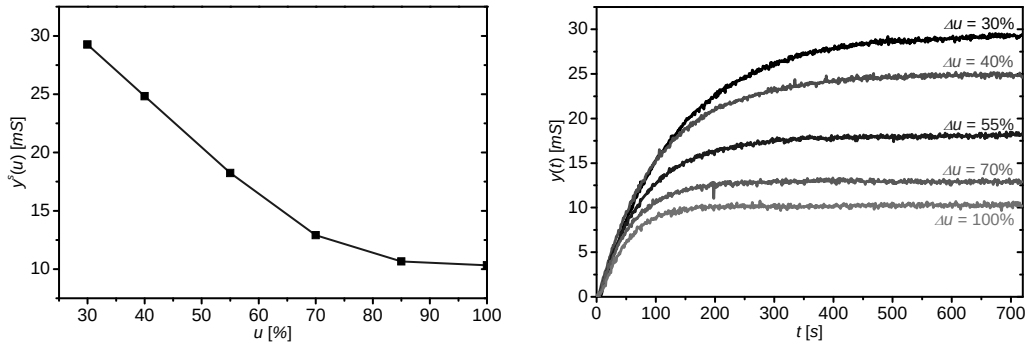


Figure 4.51 Static and dynamic analyses for the real model

Even though all responses can be described by first order transfer functions, the external linear model of this process, which is used in the control analysis, is of the second order with relative order one, i.e.

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0} \tag{4.65}$$

4.3.3 Control Analysis

Three control studies were done on this system –adaptive control with pole-placement, adaptive control with LQ and generalized predictive control (GPC).

As the results must be comparable, the same conditions were used for all measurements: sampling period T_v = 1 *s*, final time is T_f = 720 *s* (12 *min*) and three step changes of reference signal $w(t)$ during the control:

$$\begin{aligned} w(t) &= 15 \cdot [1 - \exp(-0.1 \cdot t)]\ mS \quad \text{for } t \in \langle 0; 360 \rangle\ s \\ w(t) &= 18\ mS \quad \text{for } t \in (360; 540)\ s \\ w(t) &= 14\ mS \quad \text{for } t \in \langle 540; 720 \rangle\ s \end{aligned} \tag{4.66}$$

The output variable $y(t)$ is the conductivity of the chemical in *mS* and the input variable $u(t)$ is the flow rate of clean water through pump A in %. The quality of the control is evaluated by the control quality criteria, S_u and S_y described in (4.13).

ADAPTIVE CONTROL WITH POLE-ASSIGNMENT METHOD

The adaptive control is similar as in simulation experiments – the parameters of the system are estimated recursively during the control and recomputed in each step to the parameters of the controller. Delta models were used in ELM for adaptive control and recursive identification with changing exponential forgetting were used in the parameter estimation. The starting values for the identification are:

- vector of parameters $\boldsymbol{\theta}_\delta(0) = [1.4425, -0.0141, -0.0090, -0.0033]^T$

- covariance matrix $\mathbf{P}(0) = \begin{bmatrix} 1\cdot 10^6 & 0 & 0 & 0 \\ 0 & 1\cdot 10^6 & 0 & 0 \\ 0 & 0 & 1\cdot 10^6 & 0 \\ 0 & 0 & 0 & 1\cdot 10^6 \end{bmatrix}$
- constant $K = 0.001$ and parameters $\gamma(0) = 0$, $\varepsilon(0) = 0$

The experiments have shown that the control results are much better if we impose starting values of the vector of parameters $\boldsymbol{\theta}_\delta(0)$ = [1.4425, -0.0141, -0.0090, -0.0033]^T than for arbitrary values. The values of this vector are taken from previous experiments. They could vary for each experiment but recursive identification would recompute these parameters to correct ones after some time. The second finding which follows from practical experiments is that it was good to force this vector for some time at the beginning, in our case for 50 *s*. It means that identification runs from the beginning, but the estimated parameters are taken into account from the time of 20 *s* to the end of control. The parameters from time 0-50 *s* are same as in $\boldsymbol{\theta}_\delta(0)$. The results of control are then much better and smoother on the contrary the controller without this condition ends with unacceptable results for some cases.

The transfer function of the controller for the 1DOF configuration in this case is

$$\tilde{Q}(s) = \frac{q(s)}{s\cdot\tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s\cdot(s + p_0)} \tag{4.67}$$

where the parameters of polynomials $\tilde{p}(s)$ and $q(s)$ are computed similarly as in the previous cases. The results for different values of α_i = 0.08, 0.1 and 0.3 presented in Figure 4.10 show that increasing value of α_i results in a quick output response but the input variable, $u(t)$, has a smoother course for smaller values of α_i which is considered for the pumps.

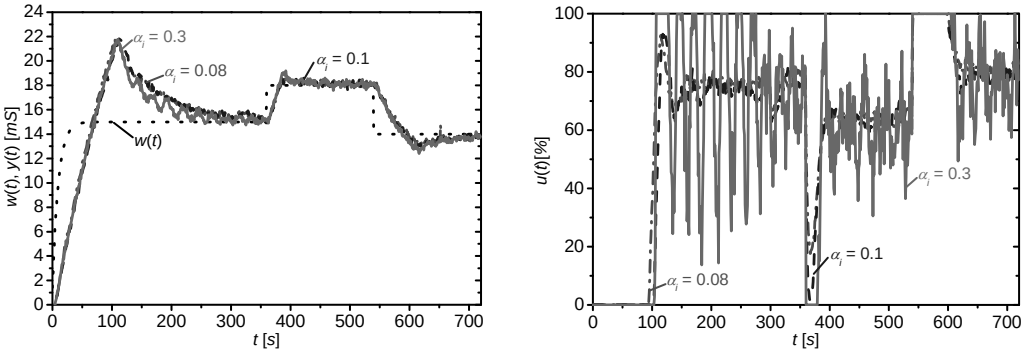


Figure 4.52 The course of $y(t)$, $w(t)$ and $u(t)$ for different positions of parameter α_i = 0.08, 0.1 and 0.3, 1DOF, pole-placement method, δ-ELM, real model

The courses of the identified parameters in Figure 4.53 show that the used identifying method has no problems with recursive estimation of unknown parameters a'_0, a'_1, b'_0 and b'_1 during whole measurement, and the estimation is relatively smooth after 100 s.

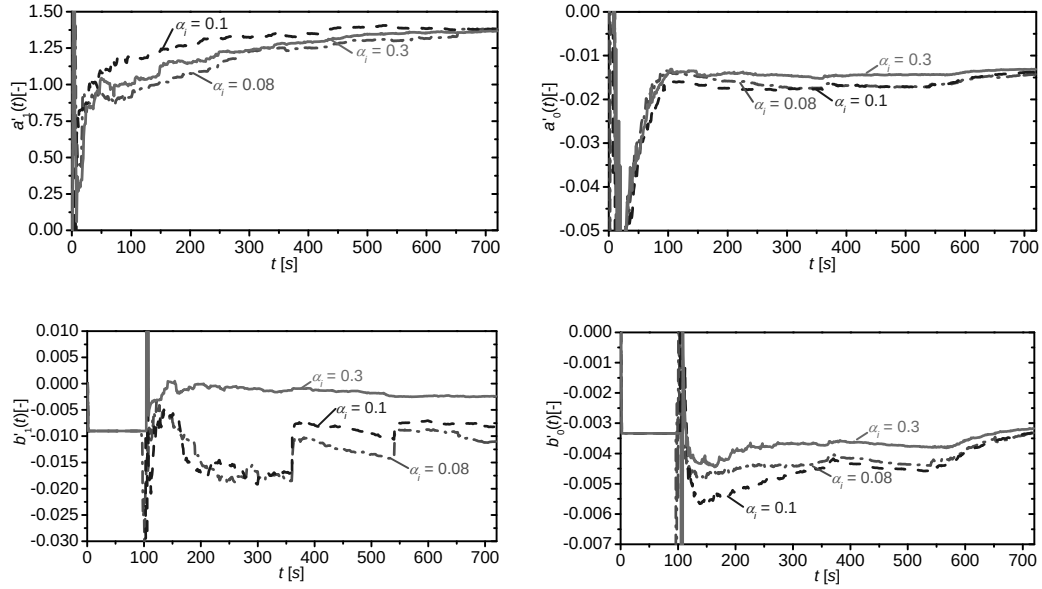


Figure 4.53 The course of identified parameters a'_0, a'_1, b'_0 and b'_1 during control, 1DOF, pole-placement method, δ-ELM, real model

The best control response according to quality criteria S_u and S_y is found for $\alpha_i = 0.08$, as can be seen in Table 4.18.

Table 4.18 The control quality crit., S_u, S_y for pole-placement method, δ-ELM, real model

	S_u[-]	S_y[-]
$\alpha_i = 0.08$	3524.8	5418.0
$\alpha_i = 0.1$	6228.4	5681.3
$\alpha_i = 0.3$	78275.0	5055.4

ADAPTIVE CONTROL WITH LQ APPROACH

The second controller was designed with the use of the LQ approach. Both 1DOF and 2DOF control configurations were used. The system is described by a second order transfer function (4.12); it means that the controllers are similar as in simulation Chapters 4.1.4 and 4.2.4. Transfer functions of the controllers are then

$$\tilde{Q}(s) = \frac{q_2 s^2 + q_1 s + q_0}{s \cdot \left(s^2 + p_1 s + p_0\right)}, \tilde{R}(s) = \frac{r_0}{s \cdot \left(s^2 + p_1 s + p_0\right)} \tag{4.68}$$

The initial parameters for identification are the same as in the previous case and the identification is switched off during the initial 50 *s* again.

As written above, the LQ method is based on minimizing of the cost function, Equation (3.112), three studies for different weighting factor ϕ_{LQ} = 0.001, 0.005 and 0.01 were done. The results are shown in Figure 4.54 and Figure 4.55.

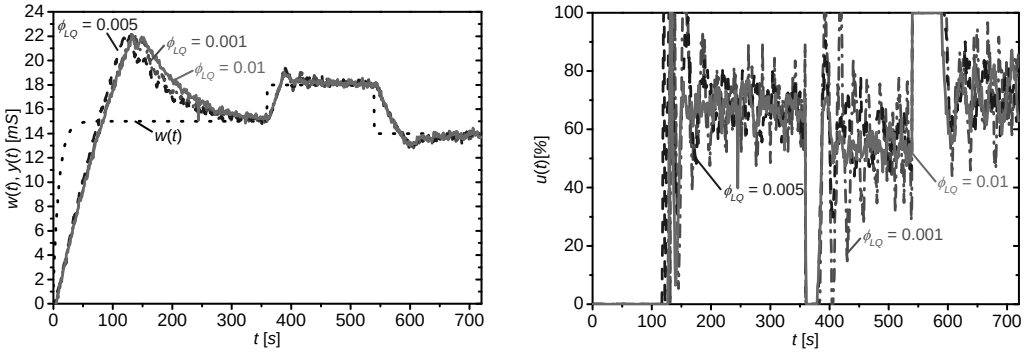


Figure 4.54 The course of $y(t)$, $w(t)$ and $u(t)$ for different positions of parameter ϕ_{LQ} = 0.001, 0.005 and 0.01, 1DOF, LQ method, δ-ELM, real model

As can be seen, the main advantage of the 2DOF configuration is that the controller can work properly from the beginning and not only after the second step change from 14 to 18 *mS* – see Figure 4.13. The value of the second weighting factor, μ_{LQ} = 1, is fixed for all studies. Again, the recursive identification has no problems with estimation.

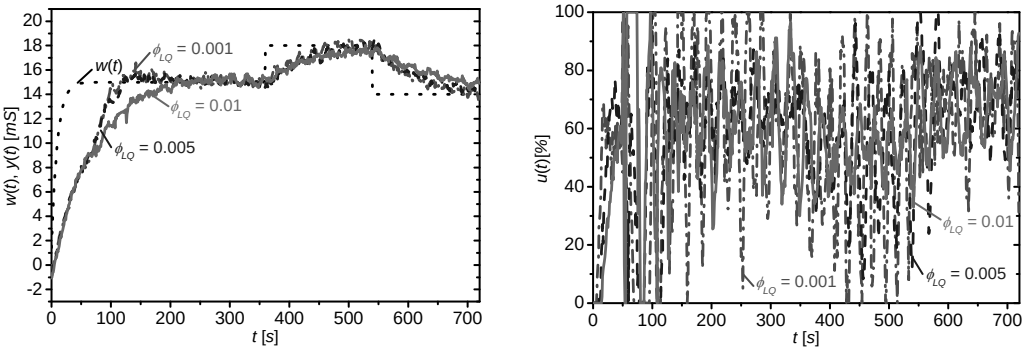


Figure 4.55 The course of $y(t)$, $w(t)$ and $u(t)$ for different positions of parameter ϕ_{LQ} = 0.001, 0.005 and 0.01, 2DOF, LQ method, δ-ELM, real model

The best setting of the controller is shown for ϕ_{LQ} = 0.005, which results in the smallest values of criteria S_u and S_y – see Table 4.19. Both configurations are compared in Figure 4.56.

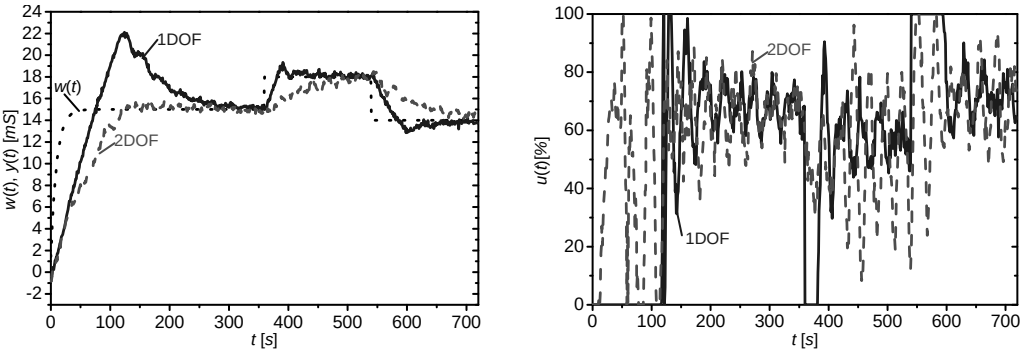


Figure 4.56 The course of $y(t)$, $w(t)$ and $u(t)$ for 1DOF and 2DOF, LQ method, $\phi_{LQ} = 0.005$, δ-ELM, real model

Table 4.19 The control quality criteria S_u, S_y for LQ method, δ-ELM, real model

	1DOF		**2DOF**	
	S_u[-]	S_y[-]	S_u[-]	S_y[-]
$\phi_{LQ} = 0.001$	83804	7018.5	94095	5843.6
$\phi_{LQ} = 0.005$	34463	6295.4	35760	5980.4
$\phi_{LQ} = 0.01$	19042	7386.0	44833	6876.0

PREDICTIVE CONTROL

The last control study uses Generalized Predictive Control (GPC). GPC technique does not use recursive identification, all we need is discrete transfer function $G(z^{-1})$:

$$G\left(z^{-1}\right) = \frac{-1.2368 \cdot 10^{-3} z^{-1} - 8.4440 \cdot 10^{-4} z^{-2}}{1 - 0.4892 z^{-1} - 0.5208 z^{-2}} \tag{4.69}$$

This transfer function was obtained as a result of discrete identification from previous control studies. The sampling period is again T_v = 1 *s*, the prediction horizon starts at N_1 = 0, ends in N_2 = 49 steps ahead, the length of the manipulation horizon is N_u = 10 steps and the first weighting factor is δ_u = 1.

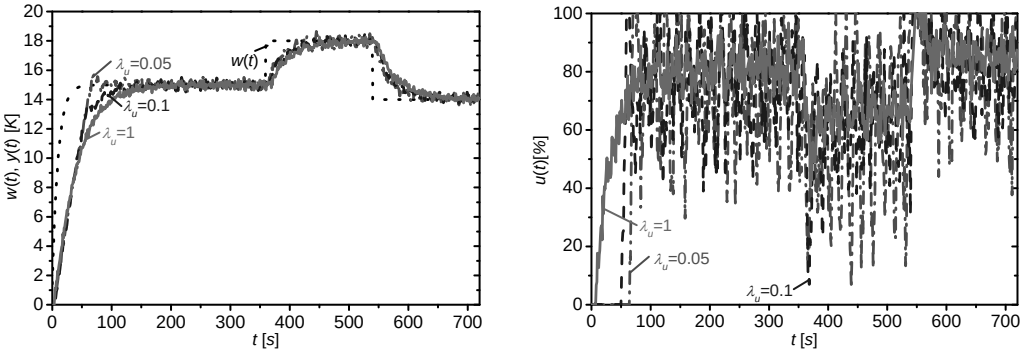


Figure 4.57 The course of $y(t)$, $w(t)$ and $u(t)$ for predictive control and different values of λ_u = 0.05, 0.1 and 1, real model

The control analyses for different weighting factor λ_u = 0.05, 0.1 and 1 are shown in Figure 4.57. Increasing value of λ_u results in a slower control response but smoother course of the manipulated variable $u(t)$, which is confirmed by the smallest value of quality criterion S_u for λ_u = 1 in Table 4.20.

Table 4.20 The control quality criteria S_u, S_y for predictive control, real model

	S_u[-]	S_y[-]
λ_u = 0.05	98784	2838.2
λ_u = 0.1	73756	3229.2
λ_u = 1	17360	3345.2

THE BEST RESULTS OF EACH CONTROL STRATEGY

All simulation studies were done for the same initial conditions, the same sampling period and the same step changes, which mean that we can now compare the best control responses of all control strategies. The results are shown in Figure 4.58 and Table 4.21. The best controllers from the controlled output $y(t)$ point of view are adaptive controller with LQ method and 2DOF configuration and GPC controller. On the other hand, the best

controller from the practical point of view, where also changes of the input variable $u(t)$ are important, is the adaptive controller with pole-placement method.

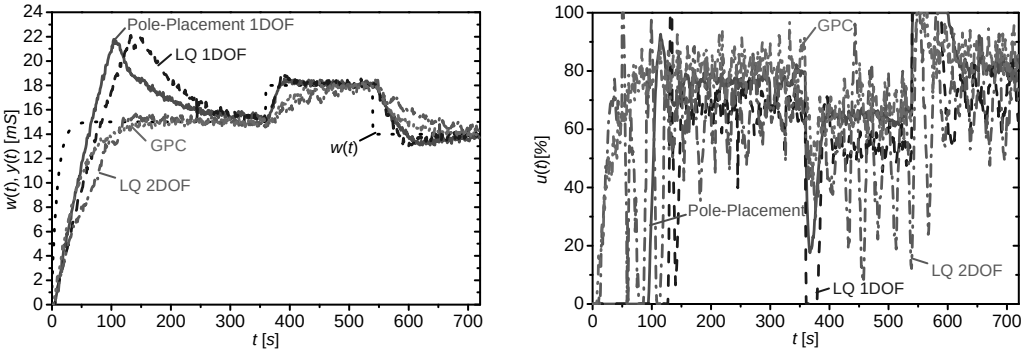


Figure 4.58 Comparison of the best control responses for Pole-placement method, LQ method and GPC

Table 4.21 The control quality criteria S_u, S_y for the best results in each control strategy

	S_u[-]	S_y[-]
Pole-placement, $\alpha_i = 0.1$	6228	5681.3
LQ 1DOF, $\phi_{LQ} = 0.005$	34463	6295.4
LQ 2DOF, $\phi_{LQ} = 0.005$	35760	5980.4
GPC, $\lambda_u = 1$	17360	3345.2

CONCLUSIONS AND DISCUSSIONS

The main objective of this work was to show the process from simulation of steady-state and dynamic analysis of different types of chemical reactors to simulation of control and verification on a real model. The chemical reactors are typical representatives of nonlinear processes, which makes them uneasy to control. However, adaptive and predictive control methods used for controlling have good control results although all models have negative control properties such as nonlinearity, time delay, non-minimum phase behaviour or changing sign of gain.

The controlled systems are first subjected to simulation analyses so that the behaviour of the system is obtained before designing the controller. The methods used for simulation in this work are mathematical modelling, steady-state and dynamic analyses. All these simulations were done in mathematical software Matlab. Although this software has build-in functions for computing the set of Ordinary Differencial Equations (functions `ode23`, `ode45`, `ode113` etc.), ODE are solved in this work with the help of Runge-Kutta's standard method programmed via equations (3.19) and (3.20) in the Chapter 3.1.4. The reason for the use of our own subfunctions is that functions `ode23`, `ode45` etc. have a variable integration step which is recomputed in according to the actual computation error and this recomputation could sometimes result in inappropriate results. On the other hand, standard Runge-Kutta's method has a fixed step, which should overcome this disadvantage. The second disadvantage of the use of functions `ode23` and `ode45` is the computation time, which is a bit longer than with the use of our own subfunction.

Simulation results will then present the behaviour of the system, which can help with the choice of the optimal working point, control strategy and design of the controller. Both control strategies, *adaptive* and *predictive Control*, were first verified simulatively and then on a real model of the CSTR.

A problem with the used Adaptive approach, which is based on the recursive identification of the External Linear Model of the originally nonlinear system, can be found at the beginning of control. The controller has not enough amount of information about the controlled system, and this results in inappropriate control responses and

overshoots, or, in the worst case, the controller does not work. However, the control response after the second and higher step change is usually much better.

One way how to overcome this problem is a use of the proportional controller for some initial time, e.g. for initial 15 steps. The input and the output have then a smooth course and the controller is fed by the initial data which reflects the behaviour of the system. The adaptive controller is switched on after these 15 steps and the controller works much more properly than without this improvement. This method was used in practical part.

The second option how to minimize the bad behaviour of the controller at the beginning is to use an exponential function for the first step change of the wanted value instead of the clean step change from the first value (usually from 0) to the second value. The reference signal then starts from zero and approaches to the final value more slowly than the clear step change.

Both methods were used in the simulation experiments but the measurements on the real model have shown that these methods cannot be used in every case. Nonlinearity and uncertainty of the controlled system cause inappropriate responses. The way of the attenuation of this goes through identified parameters from some previous measurements which are forced as a result from the recursive identification for some initial time. The identification runs from the beginning but the estimated parameters in initial 50 seconds are replaced by the parameters from a previous identification. The newly estimated parameters are used for the computation after this initial time. This improvement of the control algorithm results in stable control response because the controller does not work or works with poor results without this improvement. The use of parameters from previous measurements could evoke questions: *Why can we use these parameters for actual measurements? What will happen if we do not have the same conditions as in the previous case?* Actually, the answers to these questions are not critical for the results because the recursive identification runs independently to this intervention; moreover, this improvement the helps controller to achieve identified parameters more quickly. Different properties of the chemical could result in different parameters of ELM but the parameters taken from the previous studies are much closer to these parameters than arbitrary ones.

Interesting results in the pole-placement method are obtained with the use of spectral factorization. The parameters of the ELM could sometimes indicate unstable roots and if we choose these parameters as a part of the optional polynomial $d(s)$ on the right side of the Diophantine equations, the resulted controller is unstable too. The spectral factorization takes for designing of polynomial $d(s)$ only stable pairs of the roots and the problem with unstable controller is thus solved.

It is usually required that the controller must be tuned somehow. The optional tuning parameter in the pole-placement method with spectral factorization is position of the pole (root) α_i. The increasing value of this parameter result in quicker responses but overshoots of the output variable, as it is shown in the practical part. On the other hand, LQ technique has two tuning parameters, weighting factors μ_{LQ} and ϕ_{LQ}, and the control response depends on the ratio between these parameters. There are two cases which indicates what is important on the control process – (1) the course of the output variable $y(t)$ (ϕ_{LQ} rises with relation to the fixed μ_{LQ}) or (2) the course of the input variable $u(t)$ (ϕ_{LQ} decreases with relation to the fixed μ_{LQ}).

The use of different identification methods do not have different results – the results are in this case the same for all modifications of the Recursive least squares method with exponential or directional forgetting. Little worse results are obtained for the exponential forgetting with constant exponential forgetting but only in some cases.

The last modification of the controller is the use of different control configuration with the one degree-of-freedom (1DOF) and two degrees-of-freedom (2DOF). The simulation results and measurements on the real model have shown in some cases that 2DOF control configuration has better control results at the beginning of the control especially after the first step change when the output response from the controller with 1DOF results in overshoots while 2DOF controller has much smoother course without overshoots.

Proposed adaptive controllers have good results of the control and fulfilled basic control requirements such as the stability, the reference signal tracking and disturbance attenuation.

The best control results for all models are obtained for predictive control. The used generalized predictive control needs only two pieces of information at the beginning of control – the discrete-time transfer function, $G(z)$, of the system and weighting sequences δ_u and λ_u. The transfer function was obtained from some of the previous identifications. The predictive controller could be refined by an adaptive part where the parameters of the transfer function are identified recursively, similarly to the adaptive controller. This approach in our case does not result in better output responses but it can help with controlling of other (more complex) types of systems. The predictive control could be tuned by the choice of the ratio between parameters δ_u and λ_u similarly as for LQ control – more important is the course of the output variable $y(t)$ (λ_u rises with relation to the fixed δ_u) or the course of the input variable $u(t)$ (λ_u decreases with relation to the fixed δ_u).

The three main goals stated at the beginning of this thesis are fulfilled in 3 chapters in the following way.

1. **To perform static and dynamic analyses of different types of stirred reactors and tubular reactor.**

   The experimental part of the thesis is focused on simulation of the static and dynamic behaviour of (1) the CSTR with the so called Van der Vusse reaction A→B→C, 2A→D described by a set of four ODE, (2) the tubular chemical reactor with consecutive exothermic reaction A→B→C which mathematical model consists of a set of five partial differential equations and (3) measurement of the static and dynamic analysis on the real model of the CSTR. *This goal has been reached.*

2. **To prepare different modern control algorithms to control these chemical reactors and verify these algorithms by simulation.**

The theoretical part describes the process for constructing two types of control strategies – (1) adaptive control and (2) predictive control. The used adaptive approach is based on the choice of the ELM of the originally nonlinear process parameters of which are estimated recursively, and these parameters are then used for computation of the controller's parameters. Two control schemes were used in controller configuration – a scheme with one degree-of-freedom (1DOF) and two degrees-of-freedom (2DOF). The predictive control is based on Generalized Predictive Control, where the sequence of inputs to the controlled system is computed by minimizing of the cost function based on the sum of the control error and input variable. Both control techniques were verified on two types of chemical reactors – CSTR and tubular reactor described in the previous point. Simulations were performed for different values of the adjustable parameters of controller, position of root α_i in pole-placement method, weighting factor ϕ_{LQ} in LQ control or weighting factor λ_u in generalized predictive control, which shows the effect of this parameter to the output response from the controlled system. *This point seems to be fullfiled too.*

3. **To verify the proposed controllers from the simulation part on a real model of the continuous stirred tank reactor (CSTR)**

The last goal is connected with the verification of results from simulations to the measurements on the real model. Both adaptive and predictive approaches were used for controlling of the reactant's conductivity in the real model of CSTR. The presented output responses have shown that adaptive and predictive controllers constructed in the simulation part for different systems can be applied (with some additional measurements and settings) for this reactor, which makes them applicable for other systems. *This could be considered the main result of the thesis.*

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2) Dostal, P., Gazdos, F., Bobal, V., Vojtesek, J. Application of polznomial method in adaptive control of a CSTR. *AT&P Journal*. (accepted to publish soon)

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