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Two Degrees-of-Freedom Hybrid Adaptive Approach with Pole-placement Method Used for Control of Isothermal Chemical Reactor

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Continuous Stirred-Tank Reactors (CSTR) are technological plants often used in the chemical or biochemical industry for the production of various types of chemicals. These systems are very complex from the control point-of-view - mainly because of their nonlinearity. Controlling such processes by means of conventional methods that use controllers with fixed parameters; often produces bad - or even, unacceptable results. This is the right field for so-called “modern” control methods like Robust, Predictive, and Adaptive Control.
The control method used in this work is a hybrid adaptive control where the originally nonlinear system is represented by the external linear model whose parameters are recursively identified during the control phase. The pole-placement method with a spectral factorization and two degrees-of-freedom (2DOF) control configuration used in the control synthesis in order satisfy the basic control requirements, for instance: stability, reference signal tracking and disturbance attenuation. Moreover, the resulting controller obtained from the polynomial synthesis is easily programmable and be implemented in control computers.
All of the proposed methods were tested by simulations on a mathematical model of an isothermal CSTR, with a complex reaction inside. The results so obtained, demonstrate the applicability of this control method for these kinds of processes. The team used the MATLAB simulation program in this research.

1. Introduction

The control of chemical reactors is not a simple task - mainly due to their complexity and high nonlinearity, (Ingham et al. 2000). Conventional controllers with fixed parameters could eventually, produce inefficient output responses. That is why these systems are often-discussed subjects - and thus subjected to modern control methods like: Adaptive (Astrom and Wittenmark, 1989); Predictive (Honc, et al., 2014); Robust Control, (Grimble, 1994), etc.
Modelling and Simulation are both great tools for investigating a system’s behaviour without examining this on a real system - which could be dangerous, and demanding on time and finance resources. The mathematical model usually consists of a set of differential equations solved by the use of numerical methods like Euler’s Method or Runge-Kutta’s Method, for instance. Some of these methods are even build-in functions in the Matlab, Mathematica, and other mathematical software packages.
Various control configurations are available. The one with two degrees-of-freedom, (2DOF), (Grimble, 1994), was applied herein. The idea of Adaptive Control, (Astrom and Wittenmark, 1989), is not new but it has a great theoretical background and is still used - with various modifications and improvements on this method. Herein, the adaptive approach is based on the recursive identification of the External Linear Model (ELM), as a linear representation of a nonlinear system, (Bobal, et al., 2005). The parameters of the controller then depend on the identified ELM, and are computed in each step - using the Polynomial Method, (Kucera, 1993), or the Pole-Placement, or Spectral-factorization Methods. The result is that such approaches not only produce the controller

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that satisfies the basic control requirements; but also easily programmable relationships for computing controller's parameters - which helps with their implementation in industrial controllers.

2. Isothermal Chemical Reactor

The system under consideration is an isothermal Continuous Stirred-Tank Reactor (CSTR), (Russell and Denn, 1972) its schematic representation is shown here-below, in Figure 1.

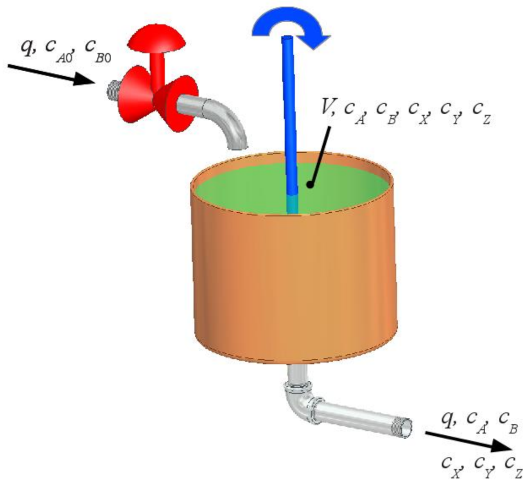


Figure 1: An Isothermal Continuous Stirred-Tank Reactor

Reactions inside a CSTR have this general form: A + B → X, A + X → Y, A + Y → Z. The mathematical model is then constructed by means of material balances. The resulting model describes these five ordinary differential equations, (Russell and Denn, 1972):

$$\begin{aligned}
\frac{dc_A}{dt} &= \frac{q}{V}\left(c_{A0}-c_A\right)-k_1\cdot c_A\cdot c_B\\
\frac{dc_B}{dt} &= \frac{q}{V}\left(c_{B0}-c_B\right)-k_1\cdot c_A\cdot c_B-k_2\cdot c_B\cdot c_X-k_3\cdot c_B\cdot c_Y\\
\frac{dc_X}{dt} &= \frac{q}{V}\left(c_{X0}-c_X\right)+k_1\cdot c_A\cdot c_B-k_2\cdot c_B\cdot c_X\\
\frac{dc_Y}{dt} &= \frac{q}{V}\left(c_{Y0}-c_Y\right)+k_2\cdot c_B\cdot c_X-k_3\cdot c_B\cdot c_Y\\
\frac{dc_Z}{dt} &= \frac{q}{V}\left(c_{Z0}-c_Z\right)+k_3\cdot c_B\cdot c_Y
\end{aligned} \tag{1}$$

It is clear that there are five State and Output Variables c_A, c_B, c_X, c_Y and c_Z; whose initial values are designated as index $c_{\cdot 0}$; the volumetric flow-rate is denoted as q; the reactor volume as V; and the reaction rate constants as k_1 – k_3. The Fixed Parameters of the reactor are shown in Table 1, (Russell and Denn, 1972).

Table 1: CSTR Fixed Parameters

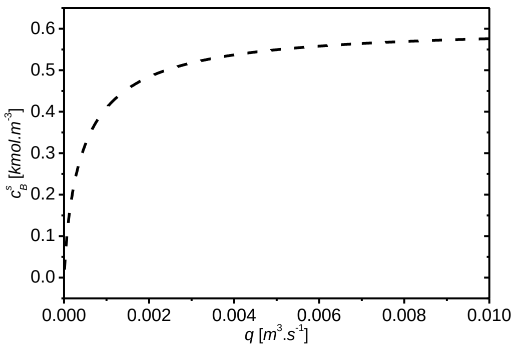
Parameter Name:	Symbol and Value	Parameter Name:	Symbol and Value
Reaction Rate Constant: 1	$k_1 = 5\times10^{-4}\ m^3.kmol^{-1}.s^{-1}$	Input Concentration of *A*:	$c_{A0} = 0.4\ kmol.m^{-3}$
Reaction Rate Constant: 2	$k_2 = 5\times10^{-2}\ m^3.kmol^{-1}.s^{-1}$	Input Concentration of *B*:	$c_{B0} = 0.6\ kmol.m^{-3}$
Reaction Rate Constant: 3	$k_3 = 2\times10^{-2}\ m^3.kmol^{-1}.s^{-1}$	*X*, *Y*, *Z* Input Concentration:	$c_{X0}=c_{Y0}=c_{Z0} = 0\ kmol.m^{-3}$
Reactor Volume:	$V = 1\ m^3$		

There is only one input variable - the volumetric flow-rate of the reactant, q - from the practical point-of-view. Steady state and dynamic analyses usually precede the design of the control and thereby help to understand the system's behavior, the choice of the working point, and the control strategy.
Theoretically, there are five output variables – the concentrations c_A, c_B, c_X, c_Y and c_Z; but, we have chosen the difference of the output concentration c_B from its initial - steady-state, value: c_B^s, as a controlled output. The

difference is there simply because the aim is that the output variable starts from zero; since the steady-state value c_B^s, is also the initial value for the dynamic study.
The input and output variables are, then:

$$y(t) = c_B(t) - c_B^s \left[kmol.m^{-3}\right] \quad u(t) = \frac{q(t) - q^s}{q^s} \cdot 100 \left[\%\right] \tag{2}$$

The steady-state analysis observes the steady-state values of concentration c_B^s for various inputs, where the volumetric flow rate: q = <0; 0.01> $m^3.s^{-1}$, is shown in the left-hand graph in Figure 2. From the dynamic analysis and control work point-of-view, the volumetric flow rate: q = 1.10^{-4} $m^3.s^{-1}$ was chosen. The dynamic analysis investigates the course of the selected output variable: y(t), after various step-changes of the input variable: u(t), from the range: u(t) = <-100%, 100%>.



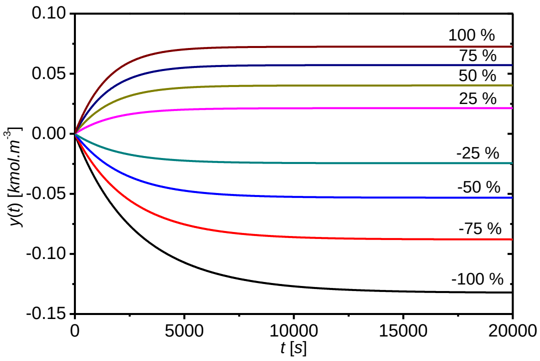


Figure 2: Steady-state Results, (Left graph); and Dynamic Analyses, (Right graph)

The mathematical solution of the steady-state means that the derivative - with respect to time, is set to be equal to 0, and the nonlinear ODE set in Eq(1) was then transformed into a set of nonlinear algebraic equations, solved by the Simple Iteration Method. The results of this analysis (in Figure 2), showed the expected nonlinear behavior of the concentration c_B. On the other hand, the dynamic analysis - represented as a numerical solution of the ODE set in Eq(1) using the Runge-Kutta's standard method - shown in the Right-hand side graph in Figure 2. A second-order Transfer Function (TF), can be used to mathematically express these output responses.

3. Hybrid Adaptive Control

In this work, Hybrid Adaptive Control is used as a control approach. The Adaptive Approach, (Astrom and Wittenmark, 1989), took its philosophy from nature, where plants, animals and even human beings "adapt" their behavior to the actual conditions of an environment. This could be done - from the control point-of-view for example, by changes to a controller's parameters, structure, etc. (Bobal, et al., 2005).
Here, the Adaptive Approach is based on the recursive identification of the External Linear Model (ELM) parameters that are recursively identified during the control process, which satisfies the exact description during the control process. Then, Polynomial Synthesis, (Kucera, 1993), is used to define the structure of the controller - and, the requisite relations for computing the controller's parameters. The following subchapters will describe the procedure for constructing such an adaptive controller.

3.1 External Linear Model (ELM)

The External Linear Model (ELM), also helps as a linear representation of what are – usually, nonlinear-systems with the selection of resultant step-responses in the Dynamic Analysis.
According to the responses - Right-hand graph in Figure 2, a second order TF was chosen as the ELM with a relative order of one; in the Polynomial form:

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0} \tag{3}$$

Where, the parameters of polynomials a(s) and b(s) are later computed from the recursive identification data and both polynomials uphold the feasibility condition for: deg a(s) ≥ deg b(s).

3.2 Controller Synthesis

A controller was designed using the Polynomial Approach, (Kucera, 1993), and a control-system configuration with two degrees-of-freedom: (2DOF), (Grimble, 1994); shown in Figure 3.

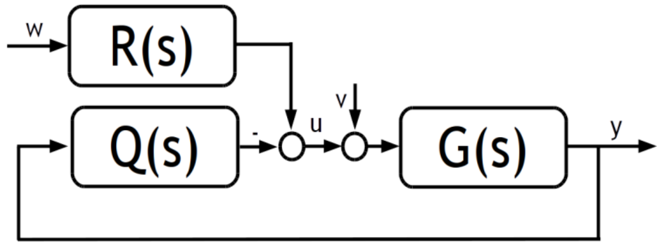


Figure 3: A Control Scheme, with two degrees-of-freedom (2DOF)

In this control configuration, the controller is divided into two parts. The first - represented by the Transfer Function Q(s), is in the feedback part; the second - the feedforward part, is in the schema denoted by the Transfer Function R(s). Then, w denotes a reference signal (wanted value); u is an input signal that is computed by the controller; v is a disturbance; and y is used for the output (controlled) signal.
The Transfer Functions of the 2DOF controller are generally:

$$Q(s)=\frac{q(s)}{p(s)};\quad R(s)=\frac{r(s)}{p(s)} \tag{4}$$

Where, the Unknown Polynomials q(s), p(s) and r(s) are – again, polynomials with the commensurable properness condition: deg p(s) ≥ deg q(s), deg p(s) ≥ deg r(s).
The reference signal tracking condition is satisfied if the polynomial p(s), in the denominator of the controller's transfer functions in Eq(4) is divided as follows:

$$p(s)=f(s)\cdot\tilde{p}(s) \tag{5}$$

Where, f(s) is the least-common divisor of the reference and the disturbance-transfer functions. If this polynomial is - for both input signals, w and v, in the range of the step function: f(s) is equal to f(s) = s, the Transfer Functions in Eq(4) are then:

$$Q(s)=\frac{q(s)}{s\cdot\tilde{p}(s)};\quad R(s)=\frac{r(s)}{s\cdot\tilde{p}(s)} \tag{6}$$

The parameters of unknown polynomials $\tilde{p}(s)$, q(s) and r(s) are computed from two Diophantine Equations, (Kucera, 1993):

$$\begin{aligned} a(s)\cdot s\cdot\tilde{p}(s)+b(s)\cdot q(s)&=d(s)\\ t(s)\cdot s+b(s)\cdot r(s)&=d(s) \end{aligned} \tag{7}$$

By means of the Uncertain Coefficients Method. Polynomials a(s) and b(s), are known from the recursive identification data and the polynomial t(s), is an auxiliary stable polynomial coefficient which is not used for computing the coefficients of the polynomial r(s). The polynomial d(s), on the right-hand side of the Diophantine Equations in Eq(7), is a stable optional polynomial that could affect control process quality. The Closed Loop system is stable if the polynomial d(s) on the left-hand side of Eq(7) is also stable.
The degrees of polynomials $\tilde{p}(s)$, q(s), r(s) and d(s) are, in the second-order TF in the ELM in Eq(3), equal to:

$$\deg\tilde{p}(s)=\deg a(s)-1=1;\ \deg q(s)=\deg a(s)=2;\ \deg r(s)=0;\ \deg d(s)=2\cdot\deg a(s)=4 \tag{8}$$

Which means that the Transfer Functions Q(s) and R(s), in (6), are:

$$Q(s)=\frac{q(s)}{s\cdot\tilde{p}(s)}=\frac{q_2 s+q_1 s+q_0}{s\cdot(p_1 s+p_0)};\quad R(s)=\frac{r(s)}{s\cdot\tilde{p}(s)}=\frac{r_0}{s\cdot(p_1 s+p_0)} \tag{9}$$

The optional polynomial d(s), on the right-hand side of the Diophantine Equations in Eq(7), chosen together with the use of the Pole-Placement Method, divides this polynomial into one - or more parts, with double, triple, etc. roots. The disadvantage of this method lies in its uncertainty – there is no general rule for the choice of these roots. Previous experiments have shown that it is good to connect this choice in some way with a controlled system. This could be - for example, by the Spectral Factorization of the polynomial a(s), in the denominator of the controlled system's Transfer Function:

$$n^{*}(s)\cdot n(s)=a^{*}(s)\cdot a(s) \tag{10}$$

where we derive a new polynomial n(s), which is - due to Spectral Factorization always being stable even if the polynomial a(s), is identified as unstable - which could happen. This polynomial is part of the d(s) that is then:

$$d(s)=n(s)\cdot(s+\alpha)^{\deg d-\deg n}=n(s)\cdot(s+\alpha)^{2} \tag{11}$$

Where the second part of this polynomial comes from the Pole-Placement Method and the Double Root $\alpha > 0$ is also a tuning parameter - which affects the course of the output variable.

3.3 On-line Identification

It previously mentioned, the computation of a controller's parameters by the Uncertain Coefficients Method needs the parameters of the system, i.e. the coefficients of polynomials a(s) and b(s) from the Transfer Function G(s). These coefficients are recursively estimated during the control process and the Recursive Least-Squares (RLS) Method, (Rao and Unbehauen, 2005), is an ideal method for this task – since it is easily programmable and could be tuned with the use of some "forgetting factor".

The on-line identification of the continuous-time model G(s) is not simple – but, this disadvantage can be overcome by using so-called "delta-models", (Middleton and Goodwin, 2004), as a special type of discrete-time models, where the input and output variables are related to the sampling period. It has been proved for example, in (Stericker and Sinha, 1993) that the parameters of the delta-model approach to the continuous one for a sufficiently small sampling period. So it is expected that - although the identification runs in discrete-time; the parameters of the delta-model are accepted as continuous ones. This approach is called "Hybrid" precisely because of this simplification.

The RLS Method then, estimates the unknown parameters from the ARX Model $y_{\delta}(k)=\hat{\theta}_{\delta}^{T}(k)\cdot\varphi_{\delta}(k\text{-}1)$ where, the data vector φ_{δ} is:

$$\begin{gathered}
y_{\delta}(k)=\frac{y(k)-2y(k-1)+y(k-2)}{T_v^2};\quad y_{\delta}(k-1)=\frac{y(k-1)-y(k-2)}{T_v};\quad y_{\delta}(k-2)=y(k-2)\\
u_{\delta}(k-1)=\frac{u(k-1)-u(k-2)}{T_v};\quad u_{\delta}(k-2)=u(k-2)
\end{gathered} \tag{12}$$

for T_v as a sampling period; and the vector of $\hat{\theta}_{\delta}$ parameters is - in this case: $\hat{\theta}_{\delta}^{T}(k)=\left[a_1^{\delta},a_0^{\delta},b_1^{\delta},b_0^{\delta}\right]^{T}$.

There are several modifications of the RLS Method with the exponential of the "directional forgetting".

4. Simulation Experiment

The hybrid adaptive controller proposed herein, was tested by simulations on the mathematical model of the Isothermal CSTR - described by the ODE set in Eq(2).

The simulation time was 30,000 s, and five step changes of the reference signal w(t) were performed during this time. As the controller has one tuning parameter α, the effect of this parameter was observed. The RLS Method - with "constant exponential forgetting", was used in this work - but previous experiments have also shown similar results for other types of "forgetting".

The Simulation Results, in Figure 4, show that the proposed control strategy deals relatively well with the task. Increasing the value of the tuning parameter α value mainly affects the speed of the control response of the output variable y(t). Lower overshoots for greater value of the parameter α can also be seen. On the other hand, lower value of α results in the smoother course of the input variable - which could be important from the practical point-of-view – the volumetric flow rate could be reduced - for example, by a twist of the valve and, quick changes of this twist could consume more energy and thus affect the service life of the equipment.

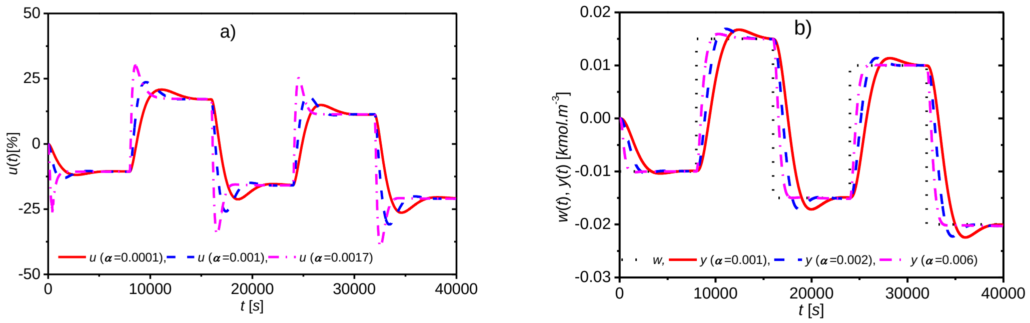


Figure 4: Courses of the input u(t) – a)*, reference signal w(t), and the output y(t) –* b)*, for different* α

5. Conclusion

This paper presents one approach to the control of Nonlinear Lumped-parameter Systems represented by an Isothermal CSTR. The mathematical model of this system is described by a set of five Nonlinear ODEs. This mathematical model was then subjected to Steady-state and Dynamic Analyses; which are, in fact, numerical solutions of the ODE set. Herein, the Control Approach is a Hybrid Adaptive Control where a controller changes its parameters according to the actual state of the system - identified during the control process by means of the RLS Method. The control system was designed in a 2DOF configuration and used together with the Polynomial Approach, the Pole-Placement Method and Spectral Factorization and satisfies basic control requirements for stability and for Reference Signal Tracking. Moreover, the resulting controller can be tuned by the choice of the root position in the Pole-Placement Method. This parameter mainly affects the speed of the control – not only in increasing the value of the root results through quicker output response, but also in quicker changes of the input variable. Simulations - performed in the Matlab mathematical software, provided all of the results. The benefit of this work can be seen in the versatility of this method – it shows an approach leading from the Steady-State and Dynamic Analysis to the Adaptive System Control. The next step is, of course, the verification on the real model in order to ensure the viability and usability of this method.

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