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# Pole placement controller with compensator adapted to semi-batch reactor process

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**Abstract:** This paper deals with the modelling and control of semi-batch reactor used for chromium sludge regeneration process. A comparison of three process control approaches is presented. Usual PID controller without online identification (OI) and adaptive PID controller were adapted to semi-batch rector process in our previous studies. In this study the two-degrees-of-freedom (2DOF) controller is developed for the same reactor control.

## 1. INTRODUCTION

Batch and semi-batch reactors are widely used in chemical, biotechnical, and pharmaceutical industries. To obtain the desired product quality during the production period an accurate temperature control is required. The temperature profile in batch and semi-batch reactors usually follows three stages (Bouhenchir et al. 2010): (i) heating of the reaction mixture up to the desired reaction temperature, (ii) maintenance of the system at this temperature and (iii) cooling stage in order to minimize the formation of by-products. Any controller used to control the reactor must be able to take into account these different stages.

In the literature some papers have been published which discuss the control of a batch or semi-batch reactor. A global linearization control strategy was applied, with online state and parameter estimation for a polymerization reactor (Beyer et al 2008). However, the authors concluded that the implementation of the proposed method is still difficult due to the missing support of required mathematical functions. The other approach was used in the next study (Cho et al. 2008), where the authors applied a dual-mode control improved by iterative learning technique. Simulations showed that the proposed method can enhance the conventional DM control with modest efforts. For rapid and suitable reference-trajectory tracking a self-adaptive predictive functional control algorithm by Škrjanc was recommended (Škrjanc 2007). This approach was successful in a reactor with switching between cold and hot water in the inlet. Neural network was applied to similar system (Wu et al. 2010) to accommodate the online identification of a nonlinear system. The authors found this strategy effective in identification and control of a class of time-varying-delayed nonlinear dynamic systems. Neural networks are often presented as a good method to reach useful results in batch processes. Some authors recommended using a tuning

parameter allowing the designer to select the damping of the closed-loop responses (Gorez 2003). A damping factor was tested in milking machine vacuum control (Reinemann 2005). Author argued that the damping factor is influenced by the system design as well as the amount of damping in the regulation device itself. Reinemann found the best value of damping factor = 1. Damping factor < 1 was causing oscillations. On the other hand, damping factor > 1 led to under-shoot. In another paper (Haugen 2005) was damping factor adjusted to the value 0,6 instead 1 for obtaining faster dynamics using Skogestad's method.

This paper presents results of experiments obtained by simulations and control of the semi-batch process using PID controller without online identification, adaptive PID controller and pole placement 2 degree-of-freedom (2DOF) controller with compensator for second order processes. The paper is organised as follows. In section 2, the semi-batch reactor and 2DOF controller are described; section 3 presents simulation results and section 4 concludes the current work and suggests new areas for investigation.

## 2. METHODS SECTION

### 2.1 The semi-batch reactor model

To simulate tanning salts from chromium sludge regeneration process a mathematical model is used. The chemical reactor scheme is shown in Fig 1. We can see there a vessel with a double wall used for a cooling liquid circulation. It has two inputs and one output. Inputs are for the cooling liquid and for the chemical compound dosing, output only for the cooling liquid.
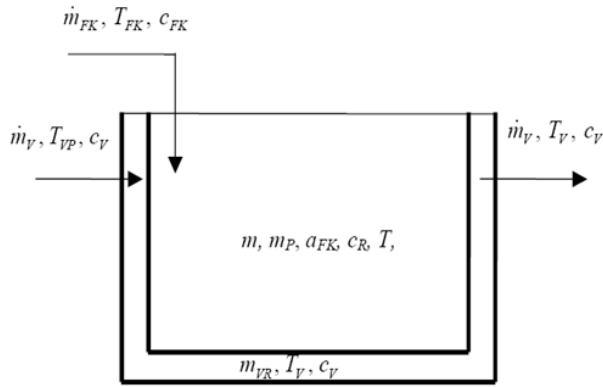
Fig. 1. Chemical reactor scheme

The mathematical model of the fed-batch reactor is defined by differential equations 1-4.

$$\dot{m}_{FK} = \frac{d}{dt} m(t) \tag{1}$$

$$\dot{m}_{FK} = k\, m(t)\, a_{FK}(t) + \frac{d}{dt}\big[m(t)a_{FK}(t)\big] \tag{2}$$

$$\dot{m}_{FK}c_{FK}T_{FK} + \Delta H_r k\, m(t)\, a_{FK}(t) = K\,S$$
$$\cdot\big[T(t) - T_V(t)\big] + \frac{d}{dt}\big[m(t)c_R T(t)\big] \tag{3}$$

$$\dot{m}_V c_V T_{VP} + K\,S\big[T(t) - T_V(t)\big] = \dot{m}_V c_V T_V(t) + m_{VR} c_V T_V'(t) \tag{4}$$

The reactor model comprises the total mass balance (1), chromium sludge mass balance, where $\dot{m}_{FK}$ is used as control signal in this process (2), the enthalpy balance (3) and coolant heat balance (4). Further variables and the parameters of the reactor model are listed in Table 1. In Eq. (2), $k$ [s$^{-1}$] is the reaction rate constant expressed by the Arrhenius equation:

$$k = Ae^{-\frac{E}{RT(t)}} \tag{5}$$

Detailed description of this model is given in Macků (2003).

*2.2 Pole placement 2 degree-of-freedom controller with compensator for second order processes*

In this work, 2DOF controller was applied to calculate the optimal temperature trajectory to reach desired properties in minimum time.
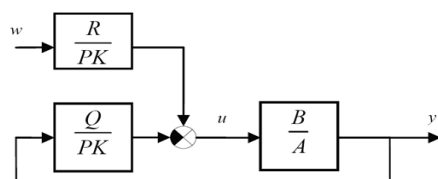


Fig. 2. 2DOF control loop

Table 1 - Variables and parameters of the reactor model

| Fig. 1 | | |
|---|---|---|
| | $m_p$ [kg] | Initial amount of reaction solution |
| (1) | $\dot{m}_{FK}$ [kg.s$^{-1}$] | Mass flow of the entering chromium sludge |
| | $m(t)$ [kg.s$^{-1}$] | Accumulation of the in-reactor content |
| (2) | $a_{FK}(t)$ [-] | Mass concentration of the chromium sludge |
| | $m(t)$ [kg] | Weight of the reaction components in the system |
| | $k$ [s$^{-1}$] | The reaction rate constant |
| (3) | $c_{FK}$ [J.kg$^{-1}$.K$^{-1}$] | Chromium sludge specific heat capacity ($c_{FK}$ = 4400 J.kg$^{-1}$.K$^{-1}$) |
| | $c_R$ [J.kg$^{-1}$.K$^{-1}$] | Reactor content specific heat capacity ($c_{FK}$ = 4500 J.kg$^{-1}$.K$^{-1}$) |
| | $T_{FK}$ [K] | Chromium sludge temperature |
| | $\Delta H_r$ [J.kg$^{-1}$] | Reaction heat ($\Delta H_r$ = 1392350 J.kg$^{-1}$) |
| | $K$ [kg$^{-3}$.K$^{-1}$] | Conduction coefficient (K = 200 kg$^{-3}$.K$^{-1}$) |
| | $S$ [m$^2$] | Heat transfer surface (S = 7,36 m$^2$) |
| | $T(t)$ [K] | Temperature of reaction components in the reactor |
| | $T_v(t)$ [K] | Temperature of coolant in the reactor double wall |
| (4) | $\dot{m}_v$ [kg.s$^{-1}$] | Coolant mass flow |
| | $c_v$ [J.kg$^{-1}$.K$^{-1}$] | Coolant specific heat capacity ($c_v$ = 4118 J.kg$^{-1}$.K$^{-1}$) |
| | $T_{vp}$ [K] | Input coolant temperature |
| | $m_{vR}$ [kg] | Coolant mass weight in the reactor double wall ($m_{vR}$ = 220 kg) |
| (5) | $A$ [s$^{-1}$] | Pre-exponential factor (A = 219,588 s$^{-1}$) |
| | $E$ [J.mol$^{-1}$] | Activation energy (E = 29967,5087 J.mol$^{-1}$) |
| | $R$ [ J.mol$^{-1}$.K$^{-1}$] | Gas constant (R = 8,314 J.mol$^{-1}$.K$^{-1}$) |

Feedback controller:

$$G_R = \frac{Q(z^{-1})}{P(z^{-1})K(z^{-1})} = \frac{q_0 + q_1 z^{-1} + q_2 z^{-2}}{(1 + p_1 z^{-1})(1 - z^{-1})} \tag{6}$$

Feedforward controller for a step reference signal:

$$G_F = \frac{R(z^{-1})}{P(z^{-1})K(z^{-1})} = \frac{r_0}{(1 + p_1 z^{-1})(1 - z^{-1})} \tag{7}$$

Characteristic polynomial of closed loop:

$$A(z^{-1})P(z^{-1})K(z^{-1}) + B(z^{-1})Q(z^{-1}) = D(z^{-1}) \tag{8}$$

Where polynomials are as follows:

$$A(z^{-1}) = 1 + \hat{a}_1 z^{-1} + \hat{a}_2 z^{-2} \qquad (9)$$

$$P(z^{-1}) = 1 + \hat{p}_1 z^{-1} \qquad (10)$$

$$K(z^{-1}) = 1 - z^{-1} \qquad (11)$$

$$B(z^{-1}) = \hat{b}_1 z^{-1} + \hat{b}_2 z^{-2} \qquad (12)$$

$$Q(z^{-1}) = q_0 + q_1 z^{-1} + q_2 z^{-2} \qquad (13)$$

$$D(z^{-1}) = 1 + d_1 z^{-1} + \ldots + d_4 z^{-4} \qquad (14)$$

$$d_1 = -2\exp(-\xi\omega T_0)\cos\left(\omega T_0 \sqrt{1 - \xi^2}\right) \qquad (15)$$

$$d_1 = -2\exp(-\xi\omega T_0)\cosh\left(\omega T_0 \sqrt{\xi^2 - 1}\right) \qquad (16)$$

$$d_2 = \exp(-2\xi\omega T_0) \qquad (17)$$

$$d_3 = d_4 = 0 \qquad (18)$$

where $\xi$ is damping factor and $\omega$ is natural frequency. Both parameters specifying dynamic behaviour of closed loop. The dynamic behaviour of the closed-loop is similar to second order continuous system with characteristic polynomial $s^2 + 2 \cdot \xi \cdot \omega \cdot s + \omega^2$.

Matrix equation:

$$\begin{bmatrix} \hat{b}_1 & 0 & 0 & 1 \\ \hat{b}_2 & \hat{b}_1 & 0 & \hat{a}_1 - 1 \\ 0 & \hat{b}_2 & \hat{b}_1 & \hat{a}_2 - \hat{a}_1 \\ 0 & 0 & \hat{b}_2 & -\hat{a}_2 \end{bmatrix} \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} d_1 + 1 - \hat{a}_1 \\ d_2 + \hat{a}_1 - \hat{a}_2 \\ d_3 + \hat{a}_2 \\ d_4 \end{bmatrix} \qquad (19)$$

Control law:

$$P(z^{-1})K(z^{-1})u_k = R(z^{-1})w_k - Q(z^{-1})y_k \qquad (20)$$

$$u_k = r_0 w_k - q_0 y_k - q_1 y_{k-1} - q_2 y_{k-2} + (1 - p_1)u_{k-1} + p_1 u_{k-2} \qquad (21)$$

$$r_0 = \frac{1 + d_1 + d_2 + d_3 + d_4}{\hat{b}_1 + \hat{b}_2} \qquad (22)$$

### 2.2 Online identification method

Proportional-integral-derivate (PID) controllers have been the most commonly used feedback controllers in the past years. The popularity and widespread use of PID controllers attributed to their simplicity and robustness but it cannot effectively control some complicated or fast running systems since the response of a plant depends on only the gain P, I and D. Most of the PID tuning rules developed in the past

years use the conventional methods. For example, the Ziegler-Nichols approach often leads to a rather oscillatory response to set-point changes because of system non-linearities and various uncertainties such as modelling error and external disturbances. These methods provide simple tuning formulae to determine the PID controller parameters. However, since only a small amount of information on the dynamic behaviour of the process is used, in many situations they do not provide good enough tuning or produce a satisfactory closed-loop response.

This was the reason to improve classical PID controller with parameters tuned according to Ziegler-Nichols from previous study (Novosad 2007). Controller was equipped by recursive least squares identification based on ARX model which can be used for the discrete on-line identification of processes described by the following transfer function:

$$G(z) = \frac{B(z^{-1})}{A(z^{-1})} = \frac{b_1 z^{-1} + b_2 z^{-2} + \ldots + b_m z^{-m}}{1 + a_1 z^{-1} + a_2 z^{-2} + \ldots + a_n z^{-n}} z^{-d} \qquad (23)$$

The estimated output of the process in the step is computed on the basis of the previous process inputs and outputs according to the equation:

$$\hat{y}_k = -\hat{a}_1 y_{k-1} - \ldots - \hat{a}_n y_{k-n} + \hat{b}_1 u_{k-d-1} + \ldots + \hat{b}_m u_{k-d-m} \qquad (24)$$

where $\hat{a}_1, \ldots \hat{a}_n, \hat{b}_1, \ldots \hat{b}_m$ are the current estimations of the process parameters. This equation can be also written in vector form, which is more suitable for further work:

$$\hat{y}_k = \Theta_{k-1}^T \cdot \Phi_k$$
$$\Phi_{k-1} = \left[\hat{a}_1, \ldots \hat{a}_n, \hat{b}_1, \ldots \hat{b}_m\right]^T \qquad (25)$$
$$\Phi_k = \left[-y_{k-1}, \ldots -y_{k-n}, u_{k-d-1}, \ldots u_{k-d-m}\right]^T$$

The vector $\Theta_{k-1}$ contains the process parameter estimations computed in the previous step and the vector $\Phi_k$ includes output and input values for computation of current output $y_k$. This on-line identification is also used for 2DOF controller.

### 3. RESULTS SECTION

Identification of suitable models which accurately describe a batch reactor process is essential to successful optimization and control. In this study, on a semi-batch reactor by means of a simulation, 2DOF controller was tested and the effect of changes of the various parameters for a quality of the regulation process was monitored.

First, $\xi$ (damping factor) coefficient was adjusted. In this aspect it must be said that some authors (Haugen 2005) introduced the recommended values of parsliameter $\xi$ around 1; however, these values were not suitable in our case. It is necessary to use a far higher value. In Fig. 3, several temperature profiles with different $\xi$ coefficients are plotted. As can be seen, the performance of the 2DOF is the best for

parameter $\xi = 45$. In cases of lower $\xi$, the setpoint is overshot (Fig 3. and Fig. 4.).

Cooling stage occurs when the reactor is full and the feeding is stopped.
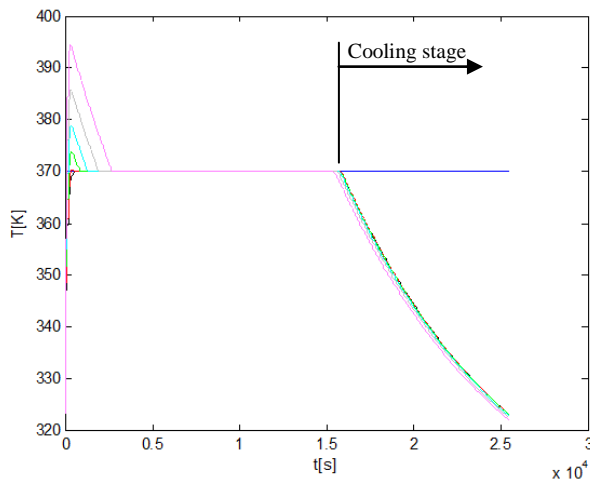


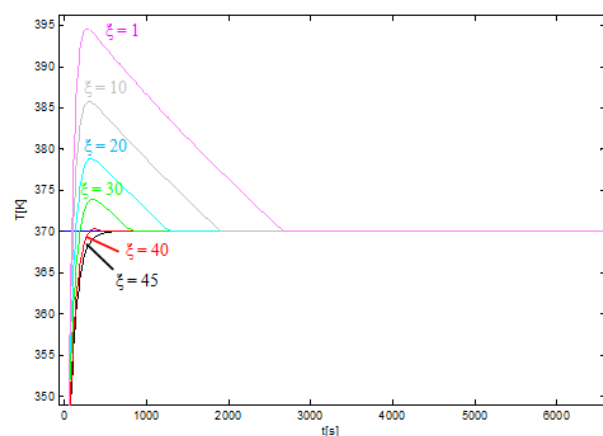Fig. 3. Comparison of the temperature profiles for different damping factor



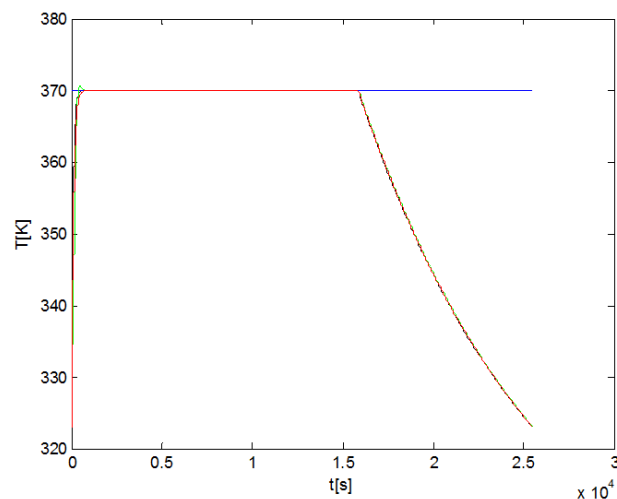Fig. 4. Comparison of the temperature profiles for different damping factor – detailed view



Fig. 5. Comparison of the temperature profiles

Figure 5 and 6 shows comparison of different methods of controlling semi-batch process. It can be seen that behaviour of PID controller without online identification and 2DOF controller are almost similar, both without oscillating and overshoots. In case of 2DOF, setpoint is reached faster for about 250 s. On the other hand, the performances in case of PID controller is slightly worse with overshoot at the beginning of the process and followed by undershoot.
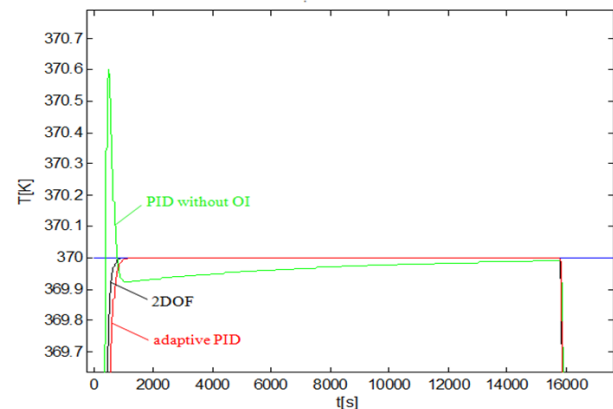


Fig. 6. Comparison of the temperature profiles – detailed view

Some differences in feeding can be also showed (Fig. 7). Maximum feeding (3 kg.s$^{-1}$) is reached in cases of controllers with online identification (adaptive PID and 2DOF). 2DOF controller provides the highest rates of the feeding at the beginning of the process and then feeding fall until the zero - feeding is stopped for about 150 s.
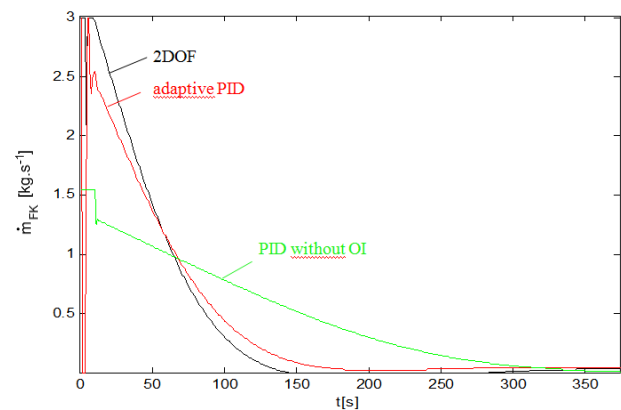


Fig. 7. Comparison of the feeding profiles at the beginning of the process

## 4. DISCUSSION SECTION

In this study, the 2DOF controller for the temperature control in a semi-batch reactor was demonstrated by simulation means. The process control sensitivity is influenced by damping factor parameter. In general it can be said that increasing of damping factor leads to reducing the overshoot and the response becomes slower. The implemented control strategy was also compared with two control strategies using

PID controllers applied on the same process in the previous works (Novosad 2007, Novosad & Macků 2010). Based on presented results it can be concluded that proposed 2DOF controller can effectively overcomes problems with oscillating around the desired value in comparison with PID controller without online identification. The quality of the regulation process in cases of controllers with implemented online identification (adaptive PID and 2DOF) shows satisfactory results.

There are still some other methods, which could possibly improve this process. In the future work, some other approaches will be applied to the batch process to find out other possible ways.

## ACKNOWLEDGMENTS

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