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.

Keywords— temperature control, online identification, semi-batch reactor, damping factor, two degrees of freedom, 2DOF

I. INTRODUCTION

LEATHER industry is perceived as a producer of pollutants in form of chrome-tanned solid waste. This waste is assuming great importance as a potential threat to human health, because it contains trivalent chromium (Cr III), which can oxidise to its hexavalent form (Cr VI) under various conditions. In tanneries, only about 20 per-cent of raw hide is transformed into the final product; the rest is waste in various forms. The best option is to recycle the chromium and return it into the tanning process or use it in other industrial processes. One of the numerous possible solutions of the problem of chrome-tanned waste is its enzymatic dechromation [1, 2].

A process of recycling chromium waste usually takes place in batch or semi-batch reactors (Fig. 1). The temperature profile during recycling operation usually follows three stages [3]: (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. For example Beyer et al. applied a global linearization control strategy with online state and parameter estimation for a polymerization reactor [4]. 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 study [5], 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 [6]. This approach was successful in a reactor with switching between cold and hot water in the inlet. Neural network was applied to similar system [7] 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.

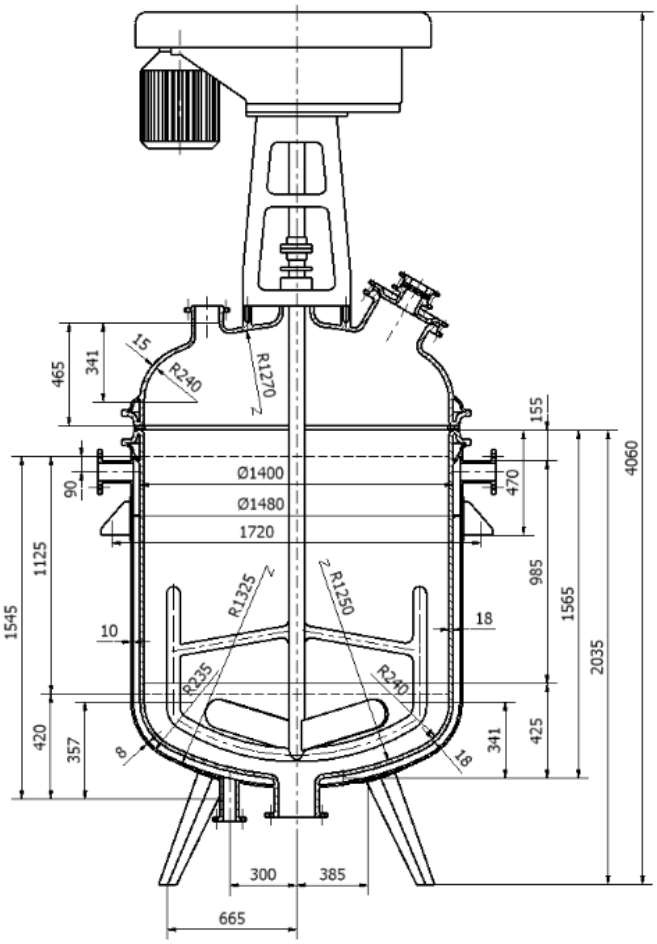

Fig. 1 Exothermic chemical semi-batch reactor

A two-degrees-of-freedom (2-DOF) decoupling control scheme was found as a satisfactory for multiple-input multiple-output (MIMO) processes with time delays [8]. A two-degree-of-freedom PI controller based on events was introduced by other author [9]. This controller is characterized by three features: the absence of clock signals in the control agents, the reduction of the number of calculated control actions, and independent tuning rules for the feed-forward and feedback parts. In the simulations and the real experiments, the performance of this new controller is very close to that of a time-triggered PI counterpart. Different approach to using two-degrees-of-freedom structure described Kleinert et al. [10]. A new cascaded control scheme was applied for batch cooling crystallizations. The advantage of this technique is precise tracking control of the main process variables by making use of respective feedforward control parts and compensation of disturbances and model uncertainties by making use of respective feedback control parts. The same structure is used to control a prototyped "smart" rotor in other study [11]. The goal of the feedback controller is to suppress the

unknown disturbances as much as possible; however, the ability to do so is limited by the requirement that the system should remain stable. A new tuning approach for two-degree-of-freedom PI controller was introduced by Nemati and Bagheri [12]. They used Butterworth rules and genetic algorithm optimization. The main advantage of proposed method is its simplicity.

Some authors recommended using a tuning parameter allowing the designer to select the damping of the closed-loop responses. Suitable value of damping can lead to satisfactory control. To develop the second order system with oscillations free response, the damping factor was used also in [13, 14]. The same coefficient was tested in a milking machine vacuum control [15] by Reinemann. Author argued that the *damping factor* is influenced by the system design as well as by the amount of damping in the regulation device itself. The best value of *damping factor* seems to be 1. *Damping factor* < 1 was causing oscillations. On the other hand, *damping factor* > 1 led to under-shoot. In other paper [16] was *damping factor* adjusted to the value 0,6 instead 1 for obtaining faster dynamics using Skogestad's method. Using of *damping factor* was also subject of investigation in our study.

The study 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.

II. Methods Section

A. The semi-batch reactor model

The chromium sludge is processed in a chemical reactor by an exothermic chemical reaction with chrome sulphate acid. In order to investigate main properties of the real process, a mathematical model simulating tanning salts from chromium sludge regeneration process is used. The chemical reactor scheme is shown in Fig 2.

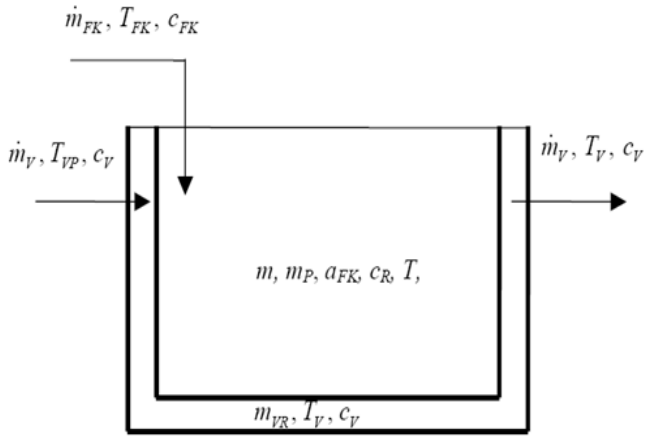

Fig. 2. Chemical reactor scheme

The mathematical model of the semi-batch reactor is defined by following 4 nonlinear ordinary differential equations:

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

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

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

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

Table I - 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 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
	ΔH_r [J.kg^{-1}]	Reaction heat (ΔH_r = 1392350 J.kg^{-1})
	K [J.m^{-2}.K^{-1}.s^{-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})

The reactor model includes four equations: the total mass balance of the chemical solution in the reactor (1), chromium sludge mass balance (2), the enthalpy balance (3) and coolant heat balance (4). Further variables and the

parameters of the reactor model are listed in Table I. In (2), $k\ [s^{-1}]$ is the reaction rate constant expressed by the Arrhenius equation:

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

Knowledge of the Arrhenius equation parameters is led to correct mathematical model, which is linked with safe and successful control [17].

B. Control theory point of view

From the system theory point of view the semi-batch reactor has four input signals $\dot{m}_{FK}(t)$, $\dot{m}_V(t)$, $T_{FK}(t)$ and $T_{VP}(t)$, four state variables $m(t)$, $a_{FK}(t)$, $T(t)$, $T_V(t)$ and one output signal to be controlled given by temperature inside the reactor $T(t)$. Hence, it can be generally seen as a multi-input multi-output system of 4th order. In addition it possesses strongly nonlinear behaviour. Practically, the only manipulated variables are input flow rates of the chromium sludge $\dot{m}_{FK}(t)$ and of the coolant $\dot{m}_V(t)$ and $T_{FK}(t)$ for batch reactor eventually. Therefore, input temperatures of the filter cake $T_{FK}(t)$ and of the coolant $T_{FK}(t)$ can be alternatively seen as disturbances, or set as a constant.

C. Ziegler-Nichols controller for second order processes with filtration of D-component using Tustin approximation (ZN2FD)

To obtain the desired quality during the production period an accurate temperature control is required. First method applied to calculate the optimal temperature trajectory to reach desired properties in minimum time was ZNFD. Control law:

$$u_k = q_0 e_k + q_1 e_{k-1} + q_2 e_{k-2} - p_1 u_{k-1} - p_2 u_{k-2} \tag{6}$$

where e_k is control error ($e_k = w_k - y_k$) and controller parameters are calculated using following equations:

$$q_o = K_P \frac{1 + 2(c_f + d_d) + \frac{c_i}{2}(1 + 2c_f)}{1 + 2c_f} \tag{7}$$

$$q_1 = K_P \frac{\frac{c_i}{2} - 4(c_f + c_d)}{1 + 2c_f} \tag{8}$$

$$q_2 = K_P \frac{c_f(2 - c_i) + 2c_d + \frac{c_i}{2} - 1}{1 + 2c_f} \tag{9}$$

$$p_I = \frac{-4c_f}{1 + 2c_f} \tag{10}$$

$$p_2 = \frac{2c_f - 1}{1 + 2c_f} \tag{11}$$

$$c_f = \frac{T_f}{T_0} \tag{12}$$

$$c_i = \frac{T_0}{T_i} \tag{13}$$

$$c_d = \frac{T_D}{T_0} \tag{14}$$

$$K_P = 0.6K_{Pu} \tag{15}$$

$$T_I = 0.5T_u \tag{16}$$

$$T_D = 0.125T_u \tag{17}$$

$$T_f = \frac{T_D}{\alpha} \tag{18}$$

where K_P, T_D and T_I are controllers parameters. In (18), α is the filtration coefficient used by filter of process output signal.

D. Pole placement 2 degree-of-freedom controller with compensator for second order processes

The other method developed in this work was 2DOF controller.

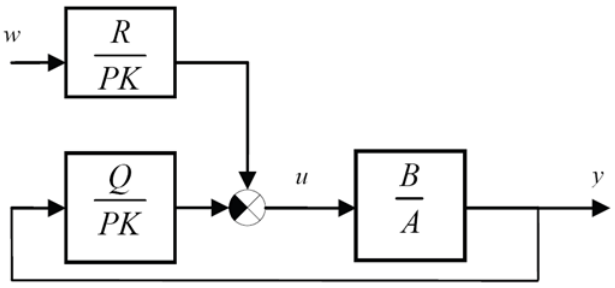

Fig. 3 2DOF control loop

Feedback controller:

$$G_R = \frac{\mathrm{Q}(z^{-1})}{\mathrm{P}(z^{-1})K(z^{-1})} = \frac{q_0 + q_1 z^{-1} + q_2 z^{-2}}{(1 + p_1 z^{-1})(1 - z^{-1})} \tag{19}$$

Feedforward controller for a step reference signal:

$$G_F = \frac{\mathrm{R}(z^{-1})}{\mathrm{P}(z^{-1})K(z^{-1})} = \frac{r_0}{(1 + p_1 z^{-1})(1 - z^{-1})} \tag{20}$$

Characteristic polynomial of closed loop:

$$A(z^{-1})P(z^{-1})K(z^{-1}) + B(z^{-1})Q(z^{-1}) = D(z^{-1}) \tag{21}$$

Where polynomials are as follows:

$$A(z^{-1}) = 1 + \hat{a}_1 z^{-1} + \hat{a}_2 z^{-2} \tag{22}$$

$$P(z^{-1}) = 1 + \hat{p}_1 z^{-1} \tag{23}$$

$$K(z^{-1}) = 1 - z^{-1} \tag{24}$$

$$B(z^{-1}) = \hat{b}_1 z^{-1} + \hat{b}_2 z^{-2} \tag{25}$$

$$Q(z^{-1}) = q_0 + q_1 z^{-1} + q_2 z^{-2} \tag{26}$$

$$D(z^{-1}) = 1 + d_1 z^{-1} + \ldots + d_4 z^{-4} \tag{27}$$

$$\mathrm{d}_1 = -2\exp(-\xi\omega \mathrm{T}_0)\cos\left(\omega \mathrm{T}_0 \sqrt{1-\xi^2}\right) \tag{28}$$

$$\mathrm{d}_1 = -2\exp(-\xi\omega \mathrm{T}_0)\cosh\left(\omega \mathrm{T}_0 \sqrt{\xi^2-1}\right) \tag{29}$$

$$\mathrm{d}_2 = \exp(-2\xi\omega \mathrm{T}_0) \tag{30}$$

$$\mathrm{d}_3 = \mathrm{d}_4 = 0 \tag{31}$$

where ξ is damping factor and ω 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:

$$\begin{bmatrix} \hat{b}_1 & 0 & 0 & 1 \\ \hat{b}_2 & \hat{b}_1 & 0 & \hat{a}_1 - 1 \\ 0 & \hat{b}_2 & \hat{b}_1 & \hat{a}_2 - \hat{a}_1 \\ 0 & 0 & \hat{b}_2 & -\hat{a}_2 \end{bmatrix} \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} d_1 + 1 - \hat{a}_1 \\ d_2 + \hat{a}_1 - \hat{a}_2 \\ d_3 + \hat{a}_2 \\ d_4 \end{bmatrix} \tag{32}$$

Control law:

$$P(z^{-1})K(z^{-1})u_k = R(z^{-1})w_k - Q(z^{-1})y_k \tag{33}$$

$$\begin{aligned} u_k &= r_0 w_k - q_0 y_k - q_1 y_{k-1} - q_2 y_{k-2} + \\ &+ (1 - p_1)u_{k-1} + p_1 u_{k-2} \end{aligned} \tag{34}$$

$$r_0 = \frac{1 + d_1 + d_2 + d_3 + d_4}{\hat{b}_1 + \hat{b}_2} \tag{35}$$

E. 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 main reason for improving classical PID controller from previous study [18]. 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:

$$G(z) = \frac{B(z^{-1})}{A(z^{-1})} = \frac{b_1 z^{-1} + b_2 z^{-2} + \ldots + b_m z^{-m}}{1 + a_1 z^{-1} + a_2 z^{-2} + \ldots + a_n z^{-n}} z^{-d} \tag{36}$$

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:

$$\begin{aligned} \hat{y}_k &= -\hat{a}_1 y_{k-1} - \ldots - \hat{a}_n y_{k-n} \\ &+ \hat{b}_1 u_{k-d-1} + \ldots + \hat{b}_m u_{k-d-m} \end{aligned} \tag{37}$$

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

$$\begin{aligned} \hat{y}_k &= \Theta_{k-1}^T \cdot \Phi_k \\ \Phi_{k-1} &= \left[\hat{a}_1, .. \hat{a}_n, \hat{b}_1, .. \hat{b}_m\right]^T \\ \Phi_k &= \left[-y_{k-1}, \ldots - y_{k-n}, u_{k-d-1}, .. u_{k-d-m}\right]^T \end{aligned} \tag{38}$$

The vector Θ_{k-1} contains the process parameter estimations computed in the previous step and the vector Φ_k includes output and input values for computation of current output y_k.

F. Recursive least square method

Least square methods are based on minimisation of the sum of prediction errors squares:

$$J_k = \sum_{i=1}^{k} (y_i - \Theta_k^T \Phi_i)^2 \tag{39}$$

where y_i is the process output in i-th step and the product $\Theta_k^T \Phi_i$ represents the predicted process output. Solving this equation leads to the recursive version of least square method where vector of parameters estimations is updated in each step according to formula:

$$\Theta_k = \Theta_{k-1} + \frac{C_{k-1} \cdot \Phi_k}{1 + \Phi_k^T \cdot C_{k-1} \cdot \Phi_k} \cdot (y_k - \Phi_{k-1}^T \Phi_k) \tag{40}$$

The covariance matrix C is then updated in each step as defined by the equation:

$$C_k = C_{k-1} + \frac{C_{k-1} \cdot \Phi_k \cdot \Phi_k^T \cdot C_{k-1}}{1 + \Phi_k^T \cdot C_{k-1} \cdot \Phi_k} \tag{41}$$

Initial value of matrix C determines the influence of initial parameter estimations on the identification process.

G. Least Square Method with exponential forgetting

The main disadvantage of this pure recursive least square method is an absence of signal weighting. Each input and output affect the result by the same weight, but actual process parameters can change in time. Thus newer inputs and outputs should affect the output more than older values. This problem can be solved by exponential forgetting method, which uses forgetting coefficient φ and decreases the weights of the data in the previous steps. Weights φ^{k-1} are assigned to values u_i and y_i. Parameter estimations are computed according to the following relations:

$$\Theta_k = \Theta_{k-1} + \frac{C_{k-1}\cdot\Phi_k}{\varphi + \Phi_k^T\cdot C_{k-1}\cdot\Phi_k}\cdot(y_k - \Phi_{k-1}^T\Phi_k) \quad (42)$$

$$C_k = \frac{1}{\varphi}\left(C_{k-1} - \frac{C_{k-1}\cdot\Phi_k\cdot\Phi_k^T\cdot C_{k-1}}{\varphi + \Phi_k^T\cdot C_{k-1}\cdot\Phi_k}\right) \quad (43)$$

III. 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.

Implementation of the method and all simulations is done in MATLAB/Simulink (Fig. 4). Important blocks are Controller, Reactor (all dynamics are defined here in form of differential equation), Saturation ensures the real behaviour of the feeder. It means that the feeding is between 0-3 kg/s. Switch prevents to overfill. Feeding is stopped, when the reactor is full.

The whole process lasts about 7 hours. The heating stage is very fast due to strong exothermic reaction. Setpoint is set to 370 K. After about 1,5 × 10^4 seconds a cooling stage occurs. During this period the temperature falls down to initial value (323,15 K).

Identification of suitable models which accurately describe a batch reactor process is essential to successful optimization and control. In this study three various controllers uses online identification – Least Squares Method. Here, to improve the temperature profile, the identification method was extended by exponential forgetting. In order to assess the improvement, the parameter φ influencing weights of the data from the previous steps, was changed. As can be seen in Fig. 5, the setpoint is reached very quickly without overshoot when φ = 1.It can be noticed that exponential forgetting is not applied when φ = 1; see (40-43).

(25)

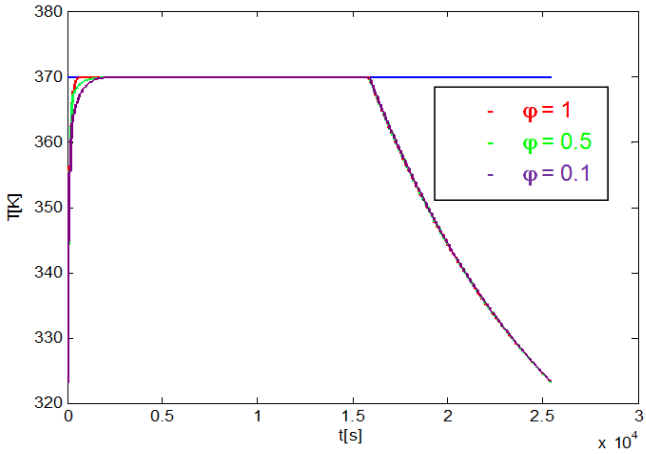

Fig. 5 Comparison of the temperature profiles for different φ coefficients

Then ξ (damping factor) coefficient was adjusted. In this aspect it must be said that some authors [16, 17] introduced the recommended values of parameter ξ around 1; however, these values were not suitable in our case. It is necessary to use a far higher value for temperature control of introduced type of nonlinear chemical semi-batch reactor. In Fig. 6, several temperature profiles with different

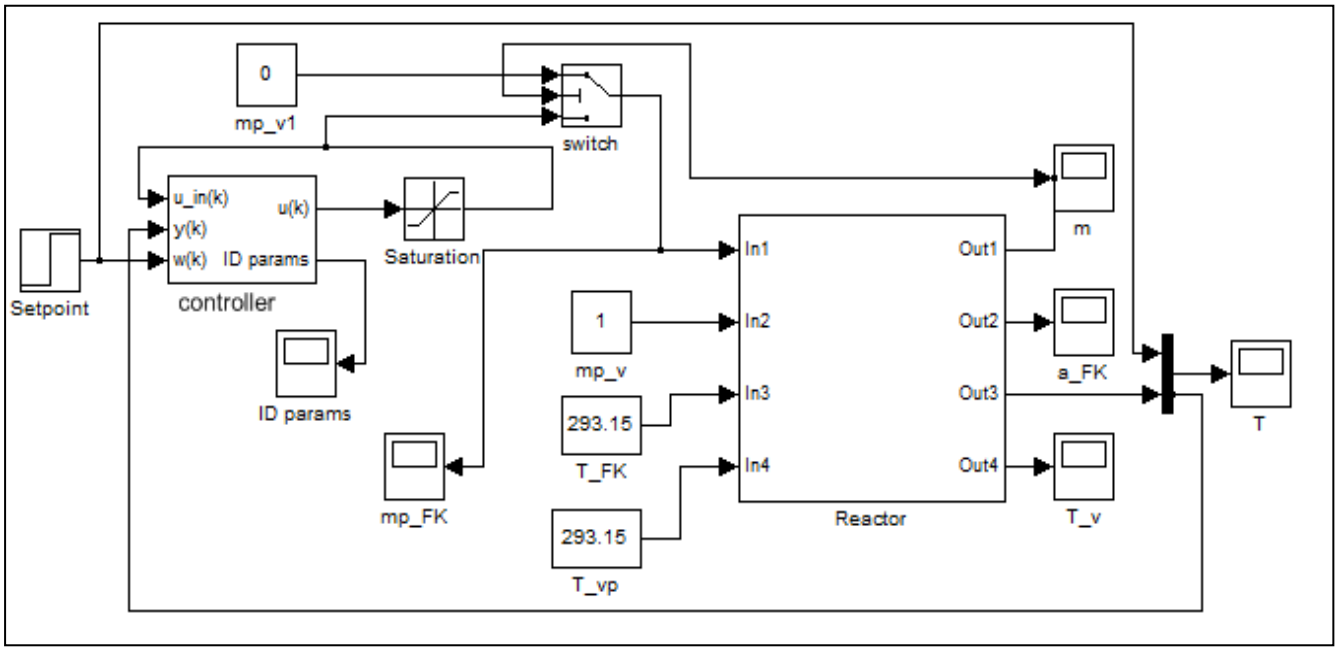

Fig. 4 Matlab Simulink scheme of controlling with 2DOF controller

ξ coefficients are plotted. As can be seen, the performance of the 2DOF is the best for parameter $\xi = 45$. In cases of lower ξ, the setpoint is overshot (Fig. 6 and Fig. 7).

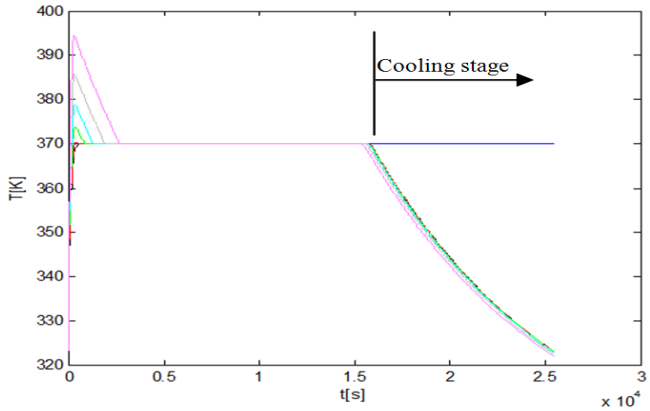

Fig. 6 Comparison of the temperature profiles for different damping factor

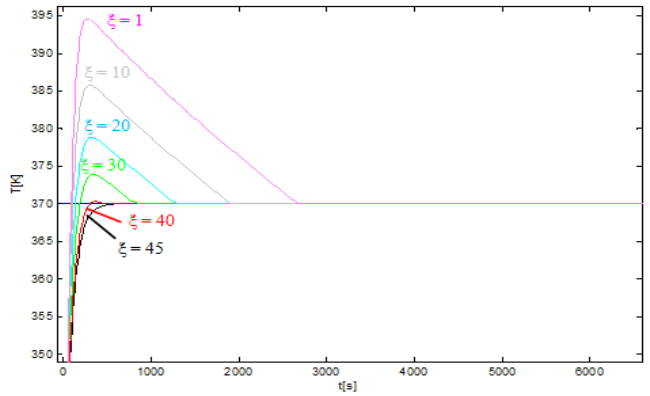

Fig. 7 Comparison of the temperature profiles inside the reactor for different damping factor – detailed view

Figure 8 and 9 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 similar, both without oscillating and overshoots. In case of 2DOF, the 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.

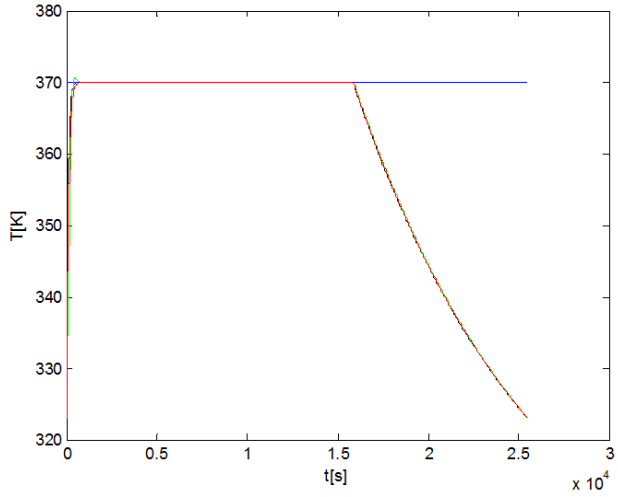

Fig. 8 Comparison of the temperature profiles inside the reactor

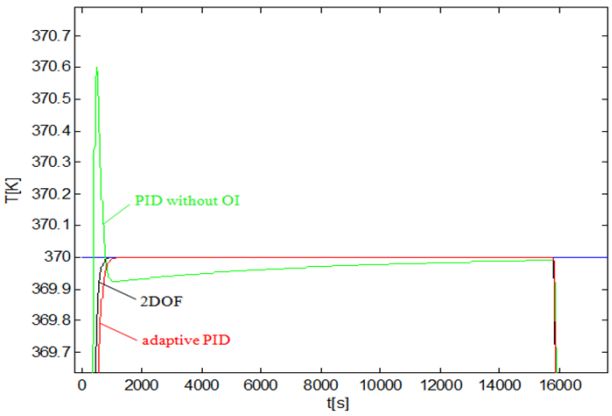

Fig. 9 Comparison of the temperature profiles inside the reactor – detailed view

Semi-batch reactor is equipped with mono-fluid heating/cooling jacket. The cooling medium is water. Temperatures profiles of water running through heating/cooling jacket can be seen in Fig. 10. and Fig. 11. The differences between used controlling methods were insignificant.

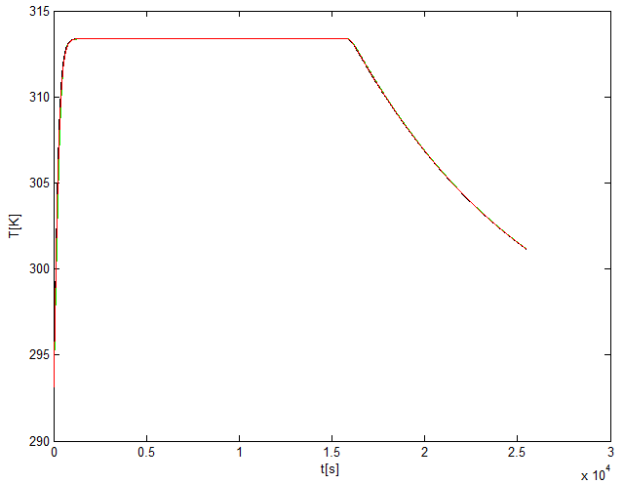

Fig. 10 Comparison of the temperature profiles of cooling water

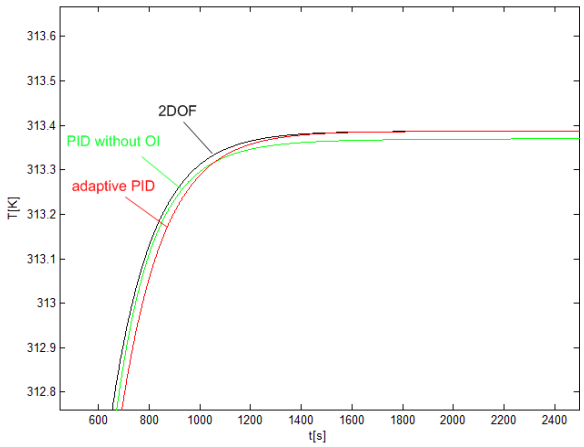

Fig. 11 Comparison of the temperature profiles of cooling water – detailed view

Mass accumulation is almost similar in all three control cases (Fig. 12). Initial amount (1810 kg) of material, including reactive solution (potassium dichromate + water + sulphuric acid) is inside the reactor at the beginning of the

process. When the reactor is full (2450 kg), feeding of chromium filter cake is stopped.

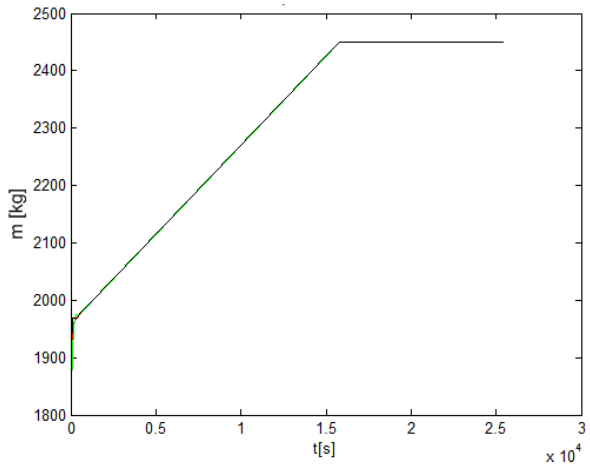

Fig. 12 Mass accumulation

Concentration of non-reacted chromium filter cake is risen at the beginning of the process then the value is established nearly zero (Fig. 13 and Fig. 14)

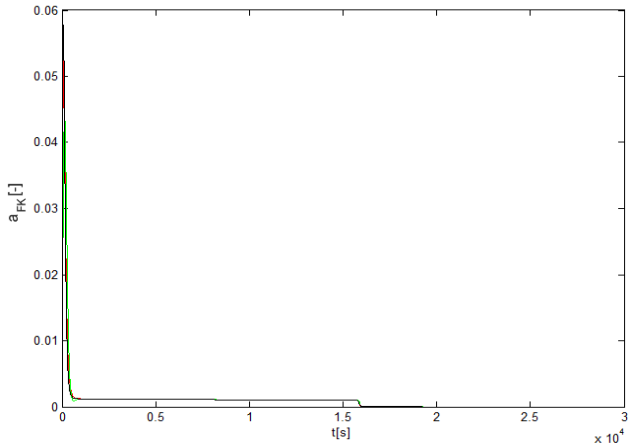

Fig. 13 Comparison of concentrations of non-reacted chromium filter cake

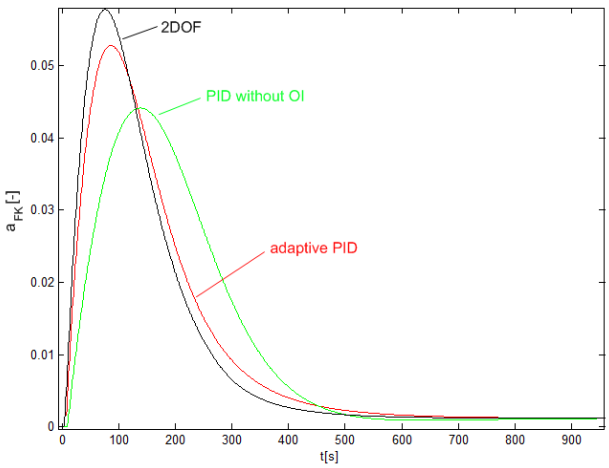

Fig. 14 Comparison of concentrations of non-reacted chromium filter cake – detailed view

Some differences in feeding can be also showed (Fig. 15). 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.

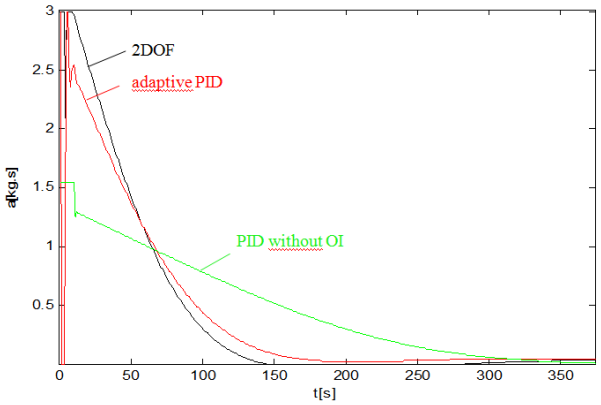

Fig. 15 Comparison of the feeding profiles at the beginning of the process (detailed view)

IV. Conclusion

In this study, the 2DOF controller for the temperature control in a semi-batch reactor was demonstrated by simulation means. The process control sensitivity in case of 2DOF controller 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 [18, 19]. 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.

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