Online identification applied on a nonlinear semi-batch process

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***Abstract*—**This paper describes the simulations of an exothermic semi batch process control. All simulations are based on a mathematical model of a real process, which runs in a semi batch reactor. The process is strongly exothermic and the temperature inside the reactor is mainly affected by the feeding speed of the chemical compound causing the reaction. Nonlinear system control is generally difficult, so it is also in this case. To tune the controller an online identification was applied. Studied were two methods, the recursive least square identification method and the same method enhanced by exponential forgetting. The mathematical simulations were performed to find an appropriate control method. Several different methods were compared to achieve the best feeding profile.

Keywords—exponential forgetting, online identification, reactor feeding, semi-batch reactor, temperature control.

I. Introduction

THE leather industry is a producer of pollutants in the form of chrome-tanned solid waste. This waste is a potential threat to human health, because it contains trivalent chromium (Cr III), which can under various conditions oxidize to its hexavalent form (Cr VI). One of the numerous possible solutions of this problem is the chrome-tanned waste enzymatic dechromation [1]. One part of the chromium waste recycling process can take place in batch or semi-batch reactors. This process releases considerable amount of heat which can endanger the reactor safety. Thus temperature control is necessary.

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 [2]: (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. Other difficulties arise because of the nonlinearities of the reactors. The important requirement of the optimal control is an accurate process model. It is necessary to know as much information as possible about this model. For this purpose, online identification can be used to identify the model parameters at the same time as the data are collected. This can lead to nonlinear systems control improvement.

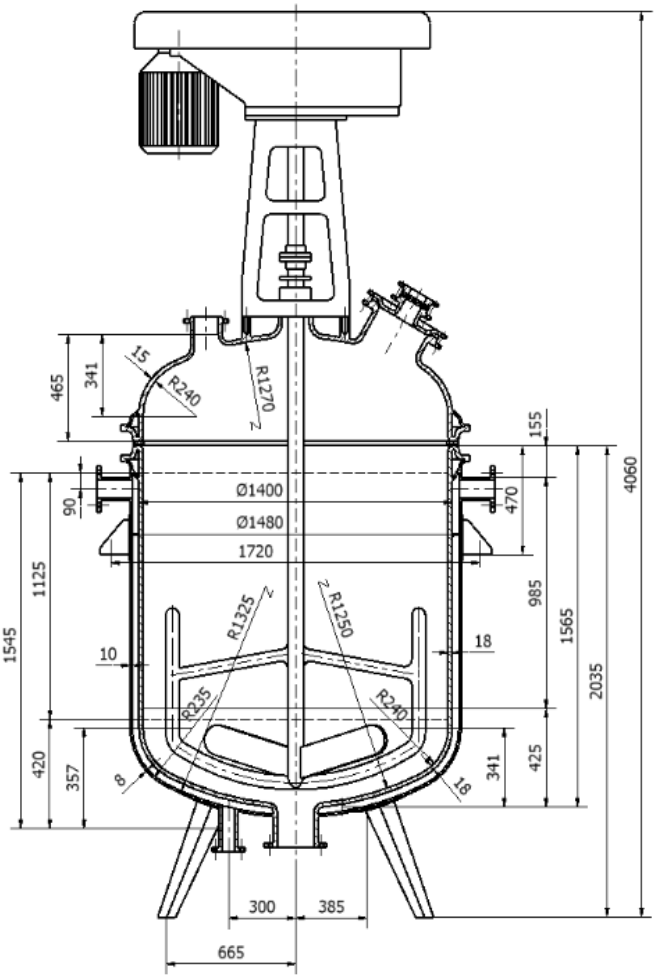

Fig. 1 Exothermic chemical semi-batch reactor

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 [3]. 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 [4], where the authors applied a dual-mode

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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 [5]. This approach was successful in a reactor with switching between cold and hot water in the inlet. Neural network was applied to similar system [6] 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. Gazdos successfully tested a robust controller with a fixed structure on our semi-batch reactor in his work [7]. An online identification of nonlinear system is then involved in work [8],[9]. Here the authors deal with online fuzzy identification and control. Inspirational publications are also [10]-[12]

The fact that hexavalent chromium in the waste generated by the leather industry could cause potential health risks is pointed out in the literature [13]. The authors' study concerns hazards of spontaneous oxidization of CrIII to CrVI in the open-air dumps and also a new three-step hybrid technology of processing manipulation waste is presented. The other study showed that the application of an elevated temperature and NaOH solution of higher concentration shorten time needed for the completely decomposition of the wastes of uncolored chromium-tanned leathers [14]. Malek et al. [15] demonstrated that chromium can be efficiently leached from the leather wastes with 0.5 M solution of potassium tartrate containing 0.25 M NaOH. The improving of chromium extraction yield of about 95% from the waste treatment was obtained according to the experimental results. The leather waste could be a useful resource and the conversion of wastes into activated carbon and fuels may be recognized as an attractive approach [16]. In this study, pyrolysis of leather wastes yielded the charred residue and ammonium carbonate besides gas and oil products.

This paper presents results of experiments obtained by real batch process simulations. These simulations involved the control of the semi-batch process using PID controller without online identification (OI), adaptive PID controller tuned using Ziegler-Nichols, the pole placement 2DOF controller with compensator for second order processes and finally PID controller tuned using pole placement method (PIDPP). The simulations results are compared with output of authors work [17]. The whole process is supposed to run in the reactor located in Kortan company in Hrádek nad Nisou [18]. Because of that fact the mathematical model was designed for this reactor, which is shown in Fig. 1.

The paper is organised as follows. In section 2, the semi-batch reactor and the ZN2FD controller with online identification 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

All simulations were performed on the nonlinear mathematical model of chromium sludge regeneration process. The semi batch process is described further. The scheme of chemical reactor used for the process is shown in Fig 2.

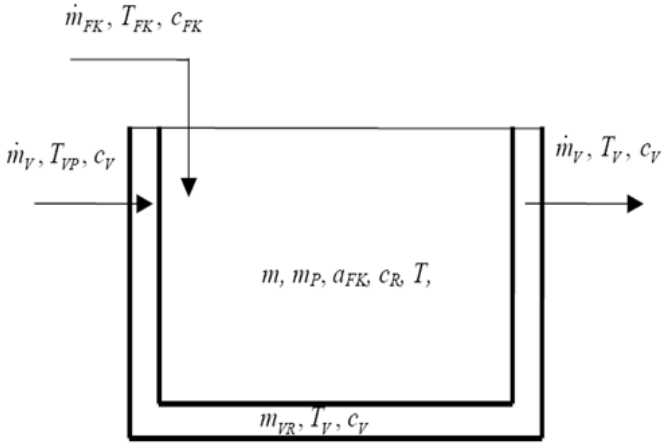

Fig. 2 Chemical reactor scheme

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

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

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

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

$$\dot{m}_V c_V T_{VP} + K\, S\left[T(t) - T_V(t)\right] = \\ = \dot{m}_V c_V T_V(t) + \frac{d}{dt}\left[m_{VR} c_V\, T(t)\right] \tag{4}$$

The reactor model comprises the total mass balance (1), chromium sludge mass balance (2), in-reactor enthalpy balance (3) and coolant enthalpy 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:

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

Table 1 - Variables and parameters of the reactor model

(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_R [J.kg^{-1}.K^{-1}]	Reactor content specific heat capacity
	T_{FK} [K]	Chromium sludge temperature
	ΔH_r [J.kg^{-1}]	Reaction heat
	K [J.m^{-2}.K^{-1}.s^{-1}]	Conduction coefficient
	S [m^2]	Heat transfer surface
	$T(t)$ [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
	T_{vp} [K]	Input coolant temperature
	m_{vR} [kg]	Coolant mass weight in the reactor double wall
(5)	A [s^{-1}]	Pre-exponential factor
	E [J.mol^{-1}]	Activation energy
	R [J.mol^{-1}.K^{-1}]	Gas constant

B. Ziegler-Nichols controller

In this work, Ziegler-Nichols controller with filtration of D-component (ZN2FD) using Tustin approximation was applied to calculate the optimal temperature trajectory to reach desired properties in minimum time. Control law of this controller can be written as:

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

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

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

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

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

$$p_I = \frac{-4c_f}{1 + 2c_f} \quad (10)$$

$$p_2 = \frac{2c_f - 1}{1 + 2c_f} \quad (11)$$

$$c_f = \frac{T_f}{T_0} \quad (12)$$

$$c_i = \frac{T_0}{T_i} \quad (13)$$

$$c_d = \frac{T_D}{T_0} \quad (14)$$

$$K_P = 0.6K_{Pu} \quad (15)$$

$$T_I = 0.5T_u \quad (16)$$

$$T_D = 0.125T_u \quad (17)$$

$$T_f = \frac{T_D}{\alpha} \quad (18)$$

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

C. Online identification

In this chapter 2 methods of online identification are mentioned. These methods can be used for the discrete on-line identification in case of processes described by the following transfer function:

$$G(z) = \frac{B(z^{-1})}{A(z^{-1})} = \frac{b_1 z^{-1} + b_2 z^{-2} + ... + b_m z^{-m}}{1 + a_1 z^{-1} + a_2 z^{-2} + ... + a_n z^{-n}} z^{-d} \quad (19)$$

The estimated output of the process in the step k ($\hat{y}_k$) is computed on the basis of the previous process inputs and outputs according to the equation:

$$\hat{y}_k = -\hat{a}_1 y_{k-1} - ... - \hat{a}_n y_{k-n} + \\ + \hat{b}_1 u_{k-d-1} + ... + \hat{b}_m u_{k-d-m} \quad (20)$$

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

$$\begin{aligned}\hat{y}_k &= \Theta_{k-1}^T \cdot \Phi_k \\ \Phi_{k-1} &= \left[\hat{a}_1,...\hat{a}_n,\hat{b}_1,...\hat{b}_m\right]^T \\ \Phi_k &= \left[-y_{k-1},...-y_{k-n},u_{k-d-1},...u_{k-d-m}\right]^T\end{aligned} \quad (21)$$

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.

D. Recursive least square method (LSM)

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

$$J_k = \sum_{i=1}^{k}(y_i - \Theta_k^T \Phi_i)^2 \quad (22)$$

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:

$$\Theta_k = \Theta_{k-1} + \frac{C_{k-1} \cdot \Phi_k}{1 + \Phi_k^T \cdot C_{k-1} \cdot \Phi_k} \cdot (y_k - \Phi_{k-1}^T \Phi_k) \quad (23)$$

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

$$C_k = C_{k-1} + \frac{C_{k-1} \cdot \Phi_k \cdot \Phi_k^T \cdot C_{k-1}}{1 + \Phi_k^T \cdot C_{k-1} \cdot \Phi_k} \quad (24)$$

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

E. LSM with exponential forgetting

The main disadvantage of the 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:

$$\Theta_k = \Theta_{k-1} + \frac{C_{k-1} \cdot \Phi_k}{\varphi + \Phi_k^T \cdot C_{k-1} \cdot \Phi_k} \cdot (y_k - \Phi_{k-1}^T \Phi_k) \quad (25)$$

$$C_k = \frac{1}{\varphi}\left(C_{k-1} \frac{C_{k-1} \cdot \Phi_k \cdot \Phi_k^T \cdot C_{k-1}}{\varphi + \Phi_k^T \cdot C_{k-1} \cdot \Phi_k}\right) \quad (26)$$

III. Results Section

This section discusses the results obtained by simulations performed on the model of semi-batch process.

A. System identification

Identification of suitable models which accurately describe a batch reactor process is essential to successful optimization and control. Also in our case an online identification was used in order to improve the quality of the control. The identification process started with initial values a_1 = 0.1, a_2 = 0.2, b_1 = 0.3, b_2 = 0.4 (Eq 20). After reaching the setpoint the parameters obtained by the system online identification stabilized at values: a_1 = -1, a_2 = 0, b_1 = 0.14, b_2 = 0.05 in case of PIDPP (Fig. 3.); a_1 = -1, a_2 = 0, b_1 = 0.17, b_2 = 0.02 in case of adaptive PID (Fig. 4.); a_1 = -1, a_2 = 0, b_1 = 0.13, b_2 = 0.044 in case of 2DOF (Fig. 5.).

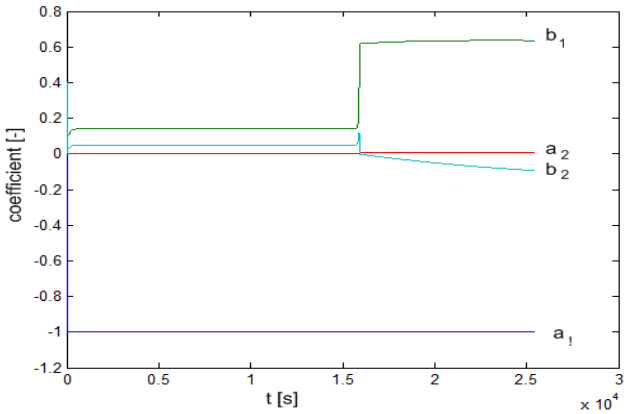

Fig. 3 Range of mathematical model parameters in case of PIDPP

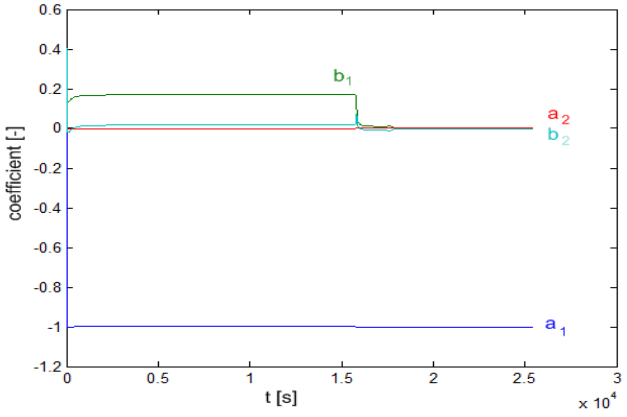

Fig. 4 Range of mathematical model parameters in case of adaptive PID

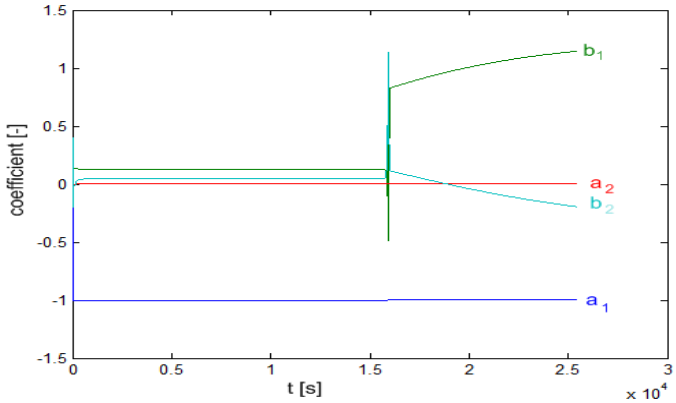

Fig. 5 Range of mathematical model parameters in case of 2DOF

B. *Influence of α coefficient*

Here α filtration coefficient of ZN2FD controller was adjusted. In this aspect it must be said that Chalupa [19] introduced the recommended values for parameter α in the range $3<\alpha<20$; however, these values were not suitable for our process. It was necessary to use a far smaller value then 3. In Fig. 6, several temperature profiles with different α filtration coefficients are plotted. The ploted α values are 0.003, 0.03, 0.3 and 3. As can be seen, the performance of the ZN2FD controller is the best for parameter α =0.003. In cases of higher α, the setpoint (in-reactor temperature) is overshot.

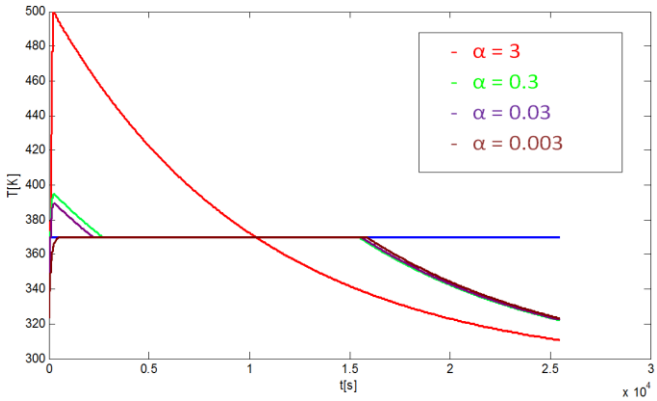

Fig. 6 Comparison of the temperature profiles for different α coefficients

C. *Identification with extended method*

In the previous section, the controller used the basic online identification method - Least squares method (LSM). Here, to improve the temperature profile, the LSM identification method was extended by exponential forgetting (LSM-EF). In order to assess the improvement, the parameter φ influencing weights of the data from the previous steps, was variously changed. As can be seen in Fig. 7, the setpoint is reached most rapidly and without overshoot when φ = 1. It can be noticed that exponential forgetting is not applied when φ = 1; see Eq. (23)-(26).

Fig. 8 shows that also the feeding profile with online identification without exponential forgetting (φ = 1) is without oscillations, unlike the other two curves. It can be said that decreasing weights of the data from the previous steps did not improve the temperature and the feeding flow rate profiles in our semi-batch reactor case.

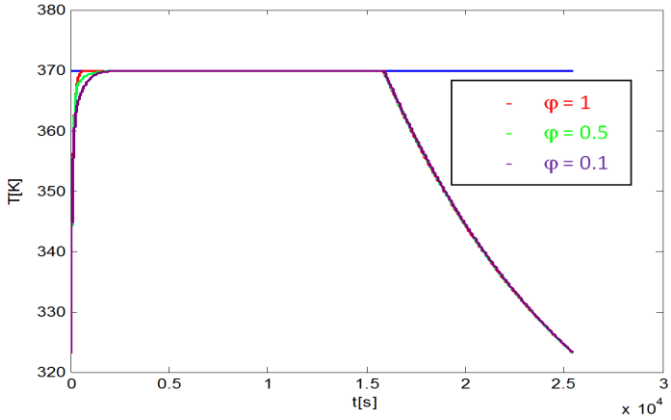

Fig. 7 Comparison of the temperature profiles for different φ coefficients

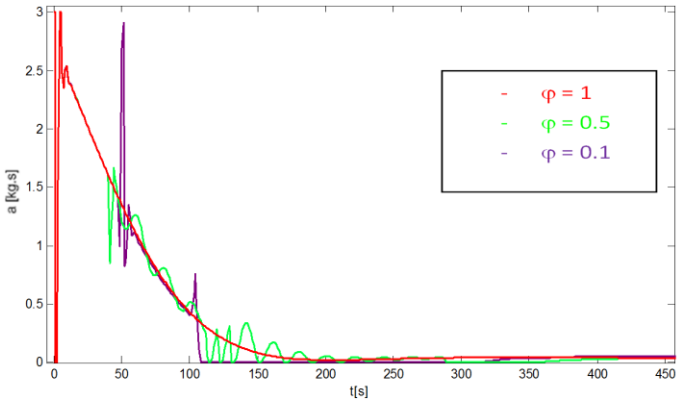

Fig. 8 Feeding profiles comparison for different φ coefficients

D. *PID controller without identification*

In previous work [17] the same semi-batch reactor was controlled by a PID controller without online identification. As can be seen from (Fig. 9) ZN2FD controller gives a better performance for temperature control. The temperature profile course is without oscillations and overshoots.

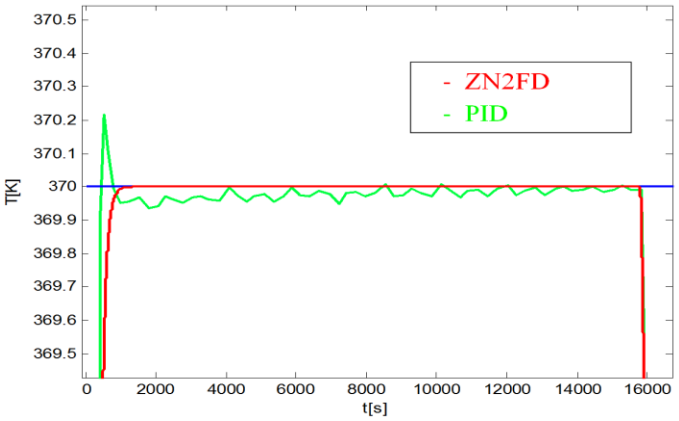

Fig. 9 Comparison of the temperature profiles between ZN2FD and PID controllers

On the other hand, feeding profile (Fig. 10) at the beginning of the control process is more suitable in the PID controller case. ZN2FD controller gives some rapid changes of feeding, which are not very suitable for actuators. However, this is valid only at the beginning of the control process. At steady state, ZN2FD controller holds constant feed rate without oscillations in contrast to PID controller (Fig. 11).

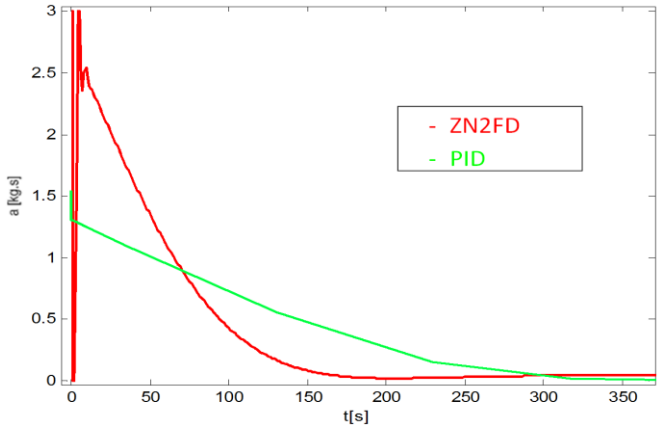

Fig. 10 Feeding profiles ZN2FD versus PID at the beginning of the process

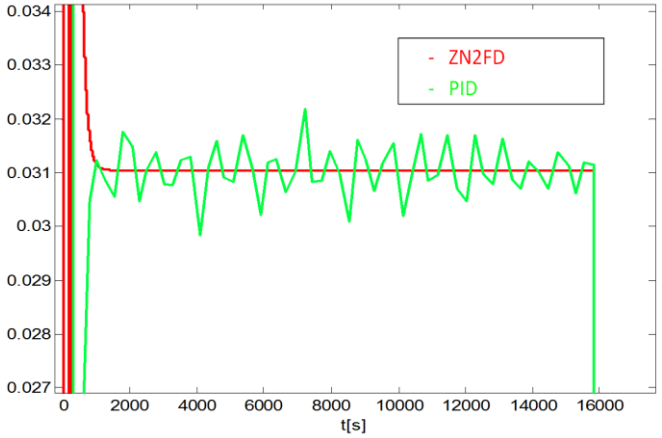

Fig. 11 Comparison of the feeding profiles between ZN2FD and PID controllers

Unfortunately, we were unable to determine why there is not direct proportionality among different values of φ coefficients (Fig. 12 and Fig. 13) and the control process. Higher φ do not speed up the process control in all cases. On the other hand, it can be concluded that there is not better value of φ than the φ = 1 for our process.

The quality of feeding can be compared in several ways. One of the most important aspects is the processing time. The faster feeding rate will lead to faster filling of the reactor and the whole process will be completed sooner. Other aspect is the in-reactor temperature. In the reactor runs strong exothermic reaction. The heat released by this reaction depends on chemical feeding. The higher feeding leads to a greater amount of the released heat. Also security aspect must be taken into consideration. The temperature inside the reactor must not exceed 100 °C. The last aspect taken into account is the smoothness of the feeding. Sudden large changes in the feeding have an adverse effect on the actuator.

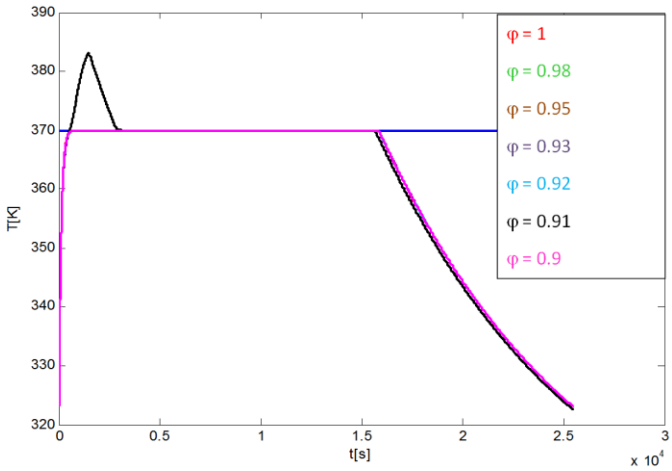

Fig. 12 Comparison of the temperature profiles for different φ coefficients

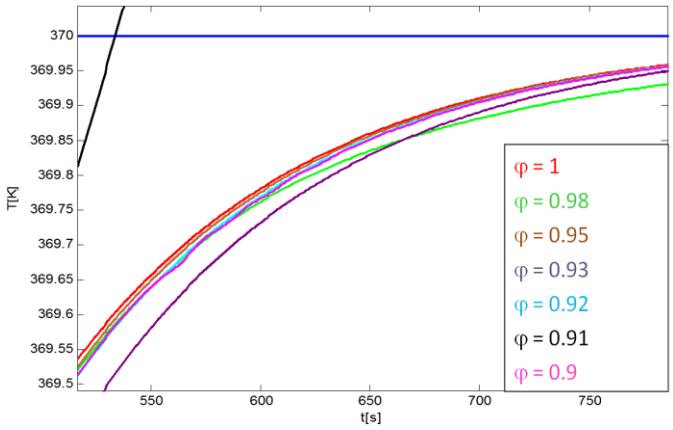

Fig. 13 Comparison of the temperature profiles for different φ coefficients – detailed view

E. Feeding profiles

Differences in feeding profiles can be observed especially at the beginning of the process. The problem is that there are two contradictory requirements. At first the in-reactor mixture must be heated-up to start the chemical reaction (i.e. feeding needs to be fast), then the feeding should be reduced (due to a large amount of the released heat) to keep the temperature under a safe border.

Fig. 14. shows feeding profile in case of PID controller without identification. As can be seen, feeding is smooth without oscillations. However, maximum possible feeding, which can be 3 kg.s-1 is not reached.

Using PIDPP controller the maximum feeding is reached. Then suddenly falls to zero and feeding is stopped for about 130 s (Fig. 15.).

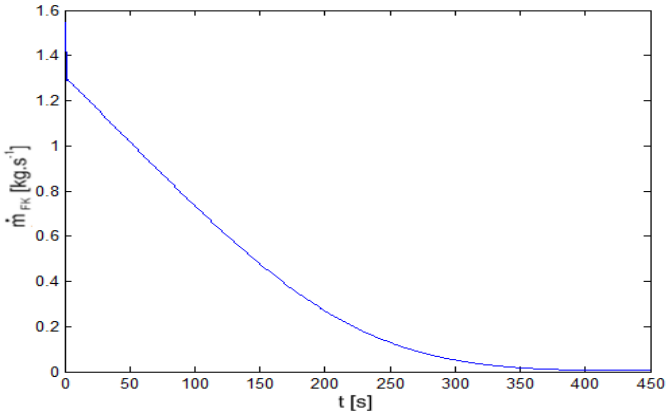

Fig. 14 PID controller feeding profile at the beginning of the process

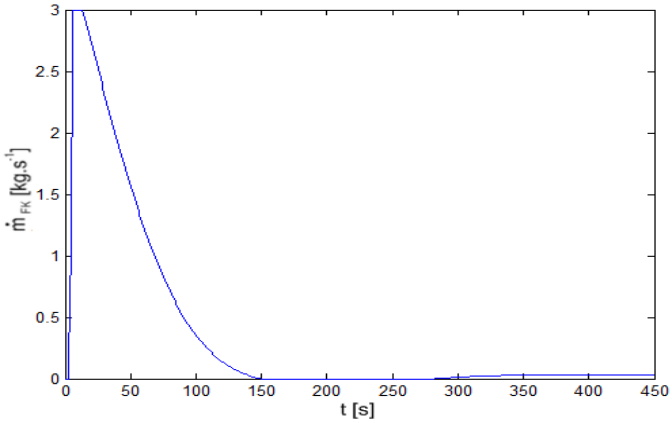

Fig. 15 PIDPP controller feeding profile at the beginning of the process

2DOF controller gives a similar result as in the previous case (Fig. 16). Feeding starts a few second earlier with small oscillations but the overall trend is the same.

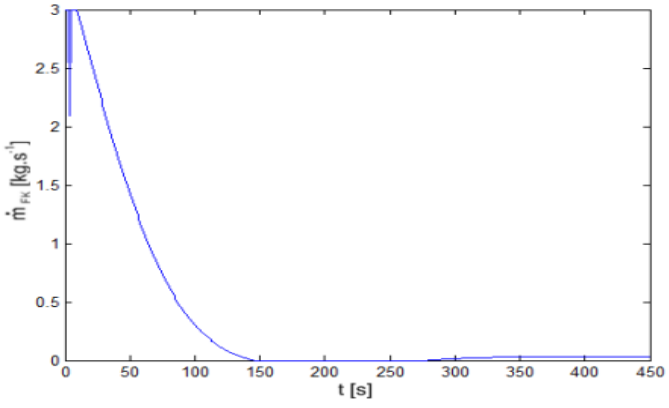

Fig. 16 2DOF controller feeding profile at the beginning of the process

As shown in Fig. 17., feeding is slowed down but not stopped in case of adaptive PID. It can be also seen some oscillations at the beginning of the process.

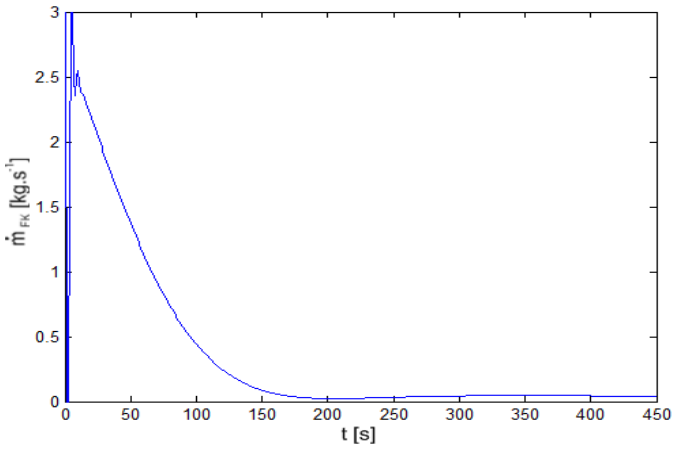

Fig. 17 Adaptive PID controller feeding profile at the beginning of the process

As can be seen in Fig. 18. each method used feeding chromium sludge in a different way.

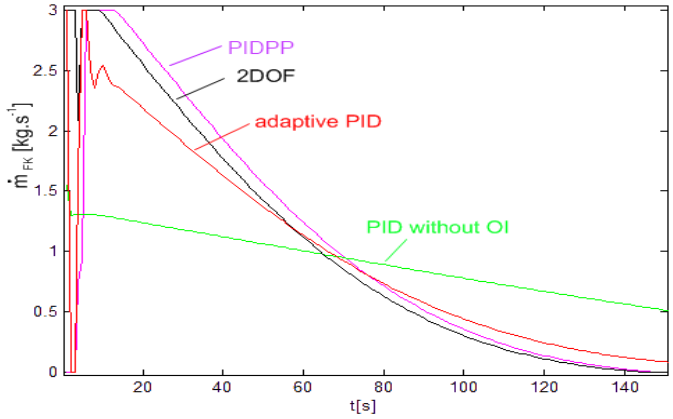

Fig. 18 Comparison of the feeding profiles at the beginning of the process

Fig. 19. and 20. show comparison of temperatures profiles throughout the whole duration of the procedure. From our perspective end time of the feeding is particularly important. The time required to fill the reactor can be seen in Table 2.

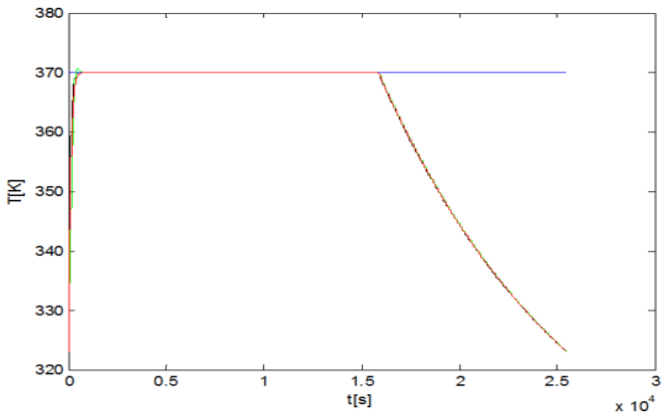

Fig. 19 Comparison of temperatures profiles

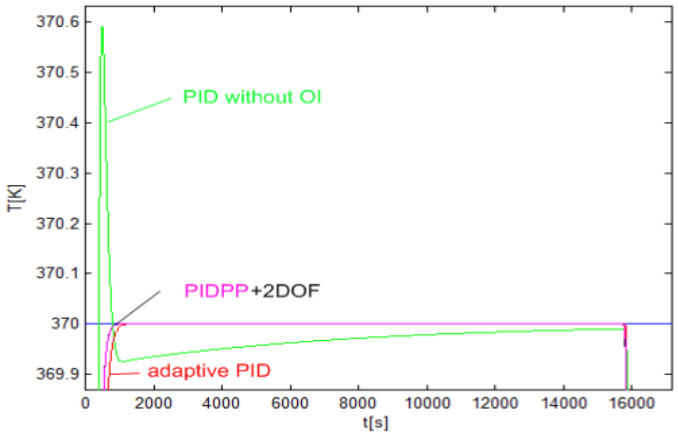

Fig. 20 Comparison of temperatures profiles – detailed view

Table 2. Comparison of the feeding time

Used method	Time of the feeding [s]
PID without OI	15 831
Adaptive PID	15 812
PIDPP	15 801
2DOF	15 799

IV. Discussion Section

Identification of suitable models which accurately describe a batch reactor process leads to successful optimization and control. In this study Ziegler-Nichols controller for second order processes with filtration of D-component (ZN2FD) was tested and the influence of various parameters changing on the quality of the control process was monitored. Also the impact of different online identification strategies was studied. Two methods of identification were tested, LSM and LSM with exponential forgetting. However, there wasn't any visible improvement for simulations using on-line identification with exponential forgetting. It may be caused by the system specific behaviour and "forgotten" data from the beginning of the control process. Therefore, it can be reported that simulation software needs all the values from previous steps for good control performance in our system.

The implemented control strategy was also compared with PID control applied on the same process in the past [14]. Based on presented results it can be concluded that proposed ZN2FD controller can effectively overcomes problems with oscillating around the desired value. In comparison with a PID controller, the ZNFD showed better quality of the control process.

In the future, the influence of a geometric arrangement and reactor dimensions on the control of the process will be studied. Also the impact of the reaction mixture composition will be monitored. Effort will be made to generalize the knowledge to any semi-batch or batch process.

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