Two step, PID and model predictive control using artificial neural network applied on semi-batch reactor

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Abstract: The article deals with the control of the semi-batch reactor that is used in chromium waste recycling process based on the enzymatic hydrolysis. The chromium waste comes from the chromium salt tanning while processing the natural leather. The recycling technique separates chrome in the form of chromium filter cake from protein. All products of this procedure are utilisable thus it is a waste free technology. The reactor deals with a problem of chromium sludge (chromium filter cake) reusing. However, the control of the semi-batch reactor is highly complex because the chemical reaction in the reactor is strongly exothermic and the in-reactor temperature is rising very fast depending on the reaction component dosing. To simulate the real process a mathematical model including reaction kinetics was used. The parameters of the achieved model were obtained and verified by experiments. Three different approaches are applied to the temperature control problem: two step control without and with penalization, PID control and model predictive control. The system control is generally difficult because of its nonlinear behaviour.

Key-Words: - Predictive control, PID control, two step control, chemical semi-batch reactor, process modelling

1 Introduction

Although the leather industry is environmentally important as a user of by-products of the meat industry, it is perceived as a consumer of resources and producer of pollutants.

The most serious problem, which is now of a great importance, is chrome-tanned solid waste. The simplest solution for this waste is its disposal in the open air. But such solution can be potentially dangerous, because uncontrolled processes in chrome waste deposited in that way could produce various soluble compounds. Chromium III (Cr III) and chromium VI (Cr VI) compounds are produced in large quantities and are accessible to most of the population. The National Institute for Occupation Safety and Health has classified the chromate and dichromate salts of calcium and magnesium (elements occurring in soil and drinking water) as carcinogenic compounds [1].

One of the numerous possible solutions of the problem of chrome-tanned waste is its enzymatic dechromation. Chrome-tanned waste in its most usual form of chromium shavings is hydrolyzed under alkali conditions in the presence of a proteolytic enzyme. After termination of the hydrolytic reaction, the hot reaction blend is filtrated. The chromium filter cake contains not only the alkali, but also a non-hydrolyzed protein. This fact can be used for the production of regenerated tanning chromium salts, which are primarily produced by the reduction of sodium dichromate with technical saccharose in a strong acid environment (sulphuric acid). By using the chromium filter cake, containing the non-hydrolyzed protein, the consumption of a relatively expensive technical saccharose is reduced [1].

Chromium filter cake (chromium sludge) processing can be done in a semi-batch reactor. Batch reactors provide flexible means of producing high value-added products in specialty chemical, biotechnical, and pharmaceutical industries. To realize the production objectives, these batch reactors have to be operated optimally in a precise fashion. However, due to the following

characteristics: 1. intrinsic nonlinearity; 2. lack of steady-state operating conditions; 3. uncertainties in reaction dynamics, or modeling error; 4. unknown disturbances; 5. constraints on process variables; 6. and limited on-line measurement information, the optimization and control of batch reactors present some of the most interesting and challenging problems for both academia and industry in the process control arena [2].

The interest in the control of batch reactors has increased in recent years because of the expansion of small-volume specialty chemicals. In the biotechnology area, batch reactors are used on both small- and largescale fermenters because of the inherent superiority of batch fermentation over continuous fermentation in most systems. Many of these batch reactors are "semibatch" or "fedbatch" reactors in which an initial amount of material is placed in the reactor, the liquid is heated to the desired temperature, and then additional feed of fresh reactant is gradually added to the vessel. The result is a time-varying process with variable volume. If heating and/or cooling is achieved by heat transfer from the vessel liquid into a heating/cooling medium in a surrounding jacket, the time-varying volume means that the heat-transfer area is also changing with time.

The optimum operation of many fed-batch reactors is an operating strategy that minimized the batch time. This corresponds to feeding the fresh feed into the reactor as quickly as possible. The feed rate is often limited by heat transfer. If the reaction is exothermic, heat must be removed. The rate of heat transfer depends on three factors [3]: 1. The temperature difference between the reaction liquid and the jacket coolant. The latter depends on the coolant flow rate, the inlet coolant temperature, and the heat-transfer rate. 2. The overall heat-transfer coefficient, which depends on agitator mixing in the vessel and the flow rate of coolant in the jacket. 3. The heat-transfer area. If jacket cooling is used, the effective heat-transfer area in a fed-batch reactor varies during the course of the batch directly with the volume of liquid in the vessel.

Due to the complexity of the reaction mixture and the difficulties to perform on-line composition measurements, control of batch and fed-batch reactors is essentially a problem of temperature control. The temperature profile in batch reactors usually follows three-stages [4]: (i) heating of the reaction mixture until 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.

2 Process model

In this paper, a fedbatch reactor model is used to study different control approaches. The model input data comes from a real process - the chromium waste recycling process [5], [6].

Let us consider single input – single output (SISO) system of chemical exothermic semi-batch reactor (figure 1). The reactor has a double wall for cooling medium and the paddle stirrer for the reaction mass stirring. As can be seen from the figure, the working area is limited by the height of the cooling double wall, thus the actual maximum working volume of the reaction mass is 2,1166 m3. The chemical reaction carried in the reactor is given by the following scheme:

$$\begin{aligned} &2C_3H_5NO + 5K_2Cr_2O_7 + Cr_2O_3 + \\ &+ 23H_2SO_4 \rightarrow 6CO_2 + N_2 + \\ &+ 28H_2O + 5K_2SO_4 + 6Cr_2(SO_4)_3 \end{aligned} \quad (1)$$

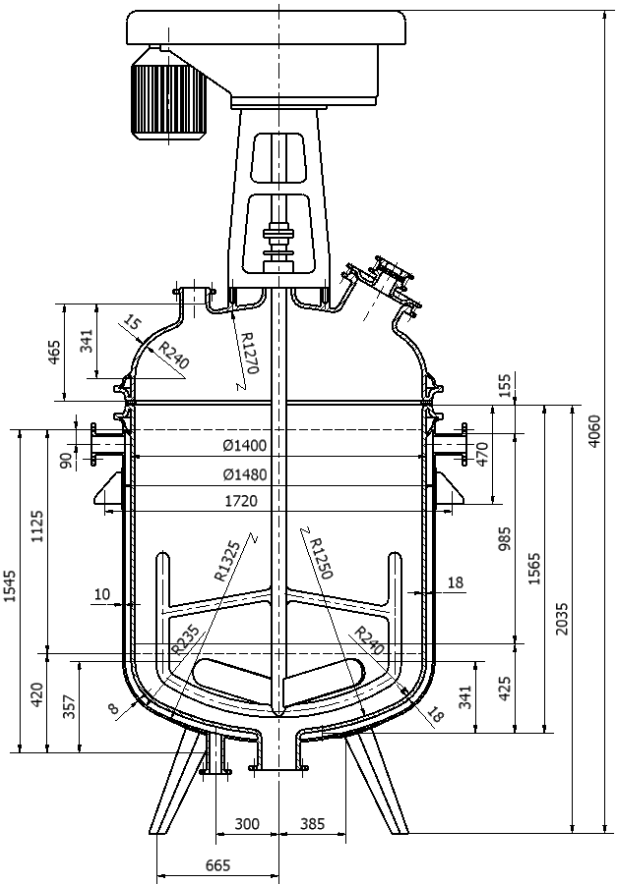

Fig. 1 Exothermic chemical semi-batch reactor.

where C_3H_5NO is the protein and Cr_2O_3 is the chromium trioxide that are main compounds of the chromium sludge. The sulphuric acid ($H_2SO_4(aq)$) and the potassium dichromate ($K_2Cr_2O_7(aq)$) are main compounds of the reactor charge. For the reactor working volume there were computed following amounts of reactants, 641.7 kg of the chromium sludge, 535.2 kg of the 96% aqueous solution of the sulphuric acid, 335.0 kg of the potassium dichromate and 940.8 kg of water. Thus, the total weight of the reactor charge is 1811.0 kg.

Water, which flows in the double wall part, is used for the cooling of the reactor. After applying usual simplifications the mathematical model of this system can be written by equations (2)-(5). The illustrative scheme of the reactor is provided in the figure 2 (where the m_B stands for weight of reactor charge).

$$\frac{\mathrm{d}\,m(t)}{\mathrm{d}\,t} = F_I \tag{2}$$

$$\frac{\mathrm{d}\,a(t)}{\mathrm{d}\,t} = \frac{F_I}{m(t)} - A \cdot e^{-\frac{E}{R \cdot T(t)}} \cdot a(t) \tag{3}$$

$$\frac{\mathrm{d}\,T(t)}{\mathrm{d}\,t} = \frac{F_I \cdot c_I \cdot T_I}{m(t) \cdot c} + \frac{A \cdot e^{-\frac{E}{R \cdot T(t)}} \cdot \Delta H_r \cdot a(t)}{c} - \frac{K \cdot S \cdot T(t)}{m(t) \cdot c} + \frac{K \cdot S \cdot T_C(t)}{m(t) \cdot c} \tag{4}$$

$$\frac{\mathrm{d}\,T_C(t)}{\mathrm{d}\,t} = \frac{F_C \cdot T_{CI}}{m_C} + \frac{K \cdot S \cdot T(t)}{m_C \cdot c_C} - \frac{K \cdot S \cdot T_C(t)}{m_C \cdot c_C} - \frac{F_C \cdot T_C(t)}{m_C} \tag{5}$$

where m is the total weight of reaction components in the reactor, a is the mass concentration of the reaction component in the reactor, c = 4500 J.kg.K^{-1} is the specific heat capacity of the reactor content, T is the temperature of the reactor content. F_I, T_I = 293.15 K and c_I = 4400 J.kg.K^{-1} is the reaction component input mass flow rate, temperature and specific heat capacity. F_C = 1 kg.s^{-1}, T_{CI} = 288.15 K, T_C, c_C = 4118 J.kg.K^{-1} and m_C = 220 kg is the cooling water mass flow rate, input temperature, output temperature, specific heat capacity and weight of the cooling water in the cooling system of the reactor, respectively. Other constants: A = 219.588 s^{-1}, E = 29967.5087 J.mol^{-1}, R = 8.314 J.mol^{-1}.K^{-1}, ΔHr = 1392350 J.kg^{-1}, K = 200 kg.s^{-3}.K^{-1}, S = 7.36 m^2.

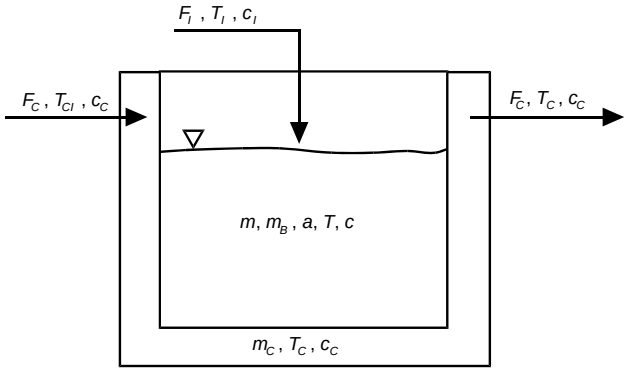

Fig. 2 Simplified scheme of exothermic chemical semi-batch reactor.

The fed-batch reactor use jacket cooling, but the effective heat-transfer area (S = 7.36 m^2) in the mathematical model was treated as constant, not time varying. The initial amount of material placed in the reactor takes about two-thirds of the in-reactor volume and the reactor is treated as ideally stirred, so we can do this simplification.

3 Control methods

Three different control methods were simulated to control the fed-batch reactor – two step control with penalization, PID control and model predictive control using artificial neural network. Also a two step control without penalization was applied, but was not satisfactory, so we skip that one. The task was to control the in-reactor temperature T by reaction component dosing F_I. The desired value of temperature T was 370K and the maximum value shouldn't exceed 373K. The actuating variable F_I was from the interval <0,3> kg.s^{-1}.

3.1 Two step control

The first control method applied on the reactor was a two step control. The actuating signal switch off was set up on 370K, switch on was set up on 365K, so the insensitivity zone was 5K. Simulations were performed for five different F_I values *{0.05; 0.1; 0.5; 1; 3}kg.s^{-1}*.

$\dot{m}_{FK}$ [kg.s^{-1}]	T_{max} [K]	T_{Vmax} [K]	a_{Fkmax} [-]	t_{total} [s]	t_{total} [h,m,s]
0,05	369,99	313,24	0,00694	27244	7, 34, 4
0,1	370,09	313,18	0,01184	26427	7, 20, 27
0,5	375,11	314,01	0,03535	25835	7, 10, 35
1	379,70	315,06	0,05291	25801	7, 10, 1
3	390,23	317,53	0,08922	25645	7, 7, 25

Table 1 Summary of values obtained by two step control

Corresponding diagrams are displayed in figures 3, 4, 5, 6. The table 1 contains summary of following data: T_{max} – the maximum reached in-reactor temperature, T_{Vmax} – maximum reached coolant temperature, a_{FKmax} – maximum in-reactor chromium sludge concentration, t_{total} – total time needed for the whole batch process.

As can be seen from the in-reactor temperature diagram in the figure 4 and from the table 1, the temperature development was satisfactory for the $F_I = \{0.05;\ 0.1\} kg.s^{-1}$ only. For higer F_I values the temperature overshoot the maximum safe value 373.15 K. On the other side, the process runs faster for higher F_I values and we need the shortest possible time. The temperature overshoot is actually caused by the reaction kinetics. The in-reactor chromium sludge concentration a_{FK} rises at the beginning of the process significantly, but the exothermic reaction is delayed because of the kinetics. After some time, the reaction starts very fast and it is impossible to stop the temperature rising because the in-reactor chromium sludge amount is already too high and caused the uncontrolled heat developing. To solve this problem, the two step control with penalization was applied on the process.

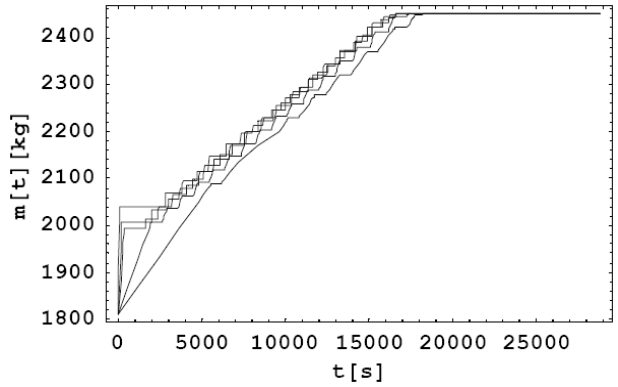

Fig. 3 The in-reactor mass development – two step control

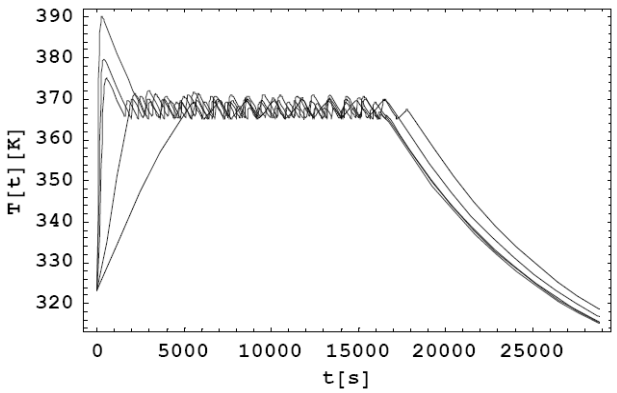

Fig. 4 The in-reactor temperature development – two step control

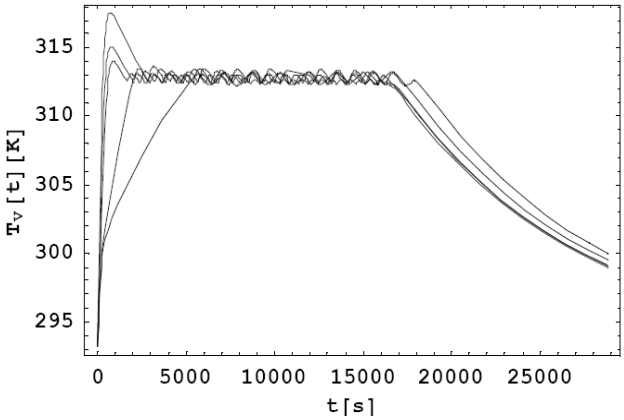

Fig. 5 The coolant temperature development – two step control

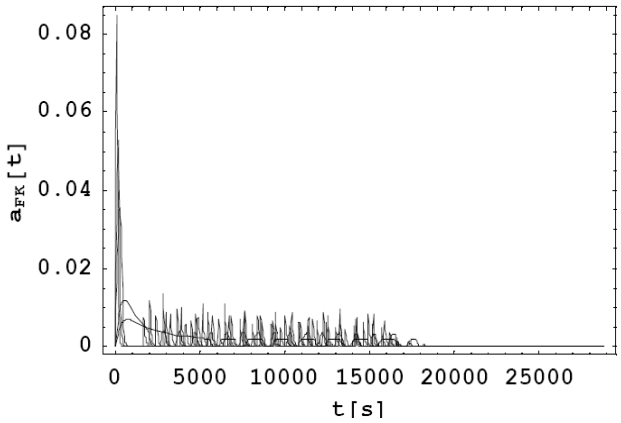

Fig. 6 The chromium sludge concentration development – two step control

3.2 Two step control with penalization

The penalization was chosen as follows – as far as the temperature exceeded the set up penalization value T_{PP} and at the same time the chromium sludge concentration was higher than the penalization value a_{FKPP}, the actuating variable F_I was switched off ($F_I = 0$). Thus was prevented the accumulation of chromium sludge in the reactor. To prevent the output value around the penalization temperature value oscillation, the insensitivity zone was chosen in the interval ($T_{PP} + 1 > T[t] \geq T_{PP}$).

Based on the simulations, the set values of penalization were following:

$F_I = 0,5$: $T_{PP} = 362K$, $a_{FKPP} = 0,02$
$F_I = 1$: $T_{PP} = 357K$, $a_{FKPP} = 0,02$
$F_I = 3$: $T_{PP} = 353K$, $a_{FKPP} = 0,02$

The simulations were carried out only for the values $F_I = \{0.5;\ 1;\ 3\} kg.s^{-1}$. Curves for the lower two values would be the same as were in two step control without penalization (there was no temperature overshoot). Corresponding diagrams with penalization are displayed in figures 7, 8, 9, 10.

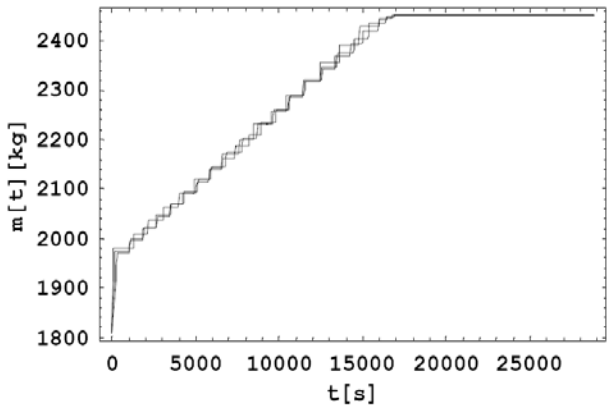

Fig. 7 The in-reactor mass development – two step control with penalization

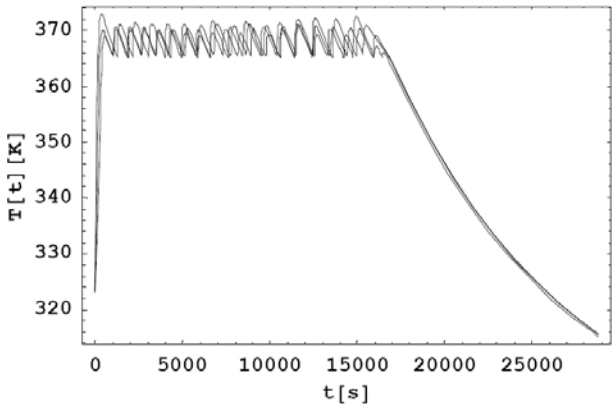

Fig. 8 The in-reactor temperature development – two step control with penalization

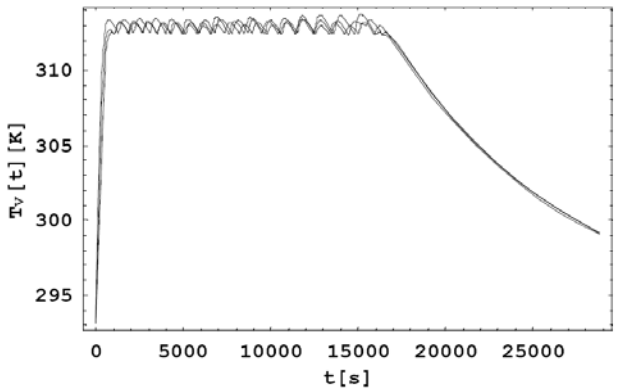

Fig. 9 The coolant temperature development – two step control with penalization

As can be seen from the in-reactor temperature development and also from table 2, the two step control with penalization was satisfactory. The in-reactor temperature did not exceed *373.15K*, the coolant temperature reached *314K*, so the control demands were fulfilled. The results shows, that the actuating variable F_1 increasing has from the $F_1 = 0.5\ kg.s^{-1}$ minimal influence on the total process time (less than three minutes from the total time of 7 hours while actuating variable was increased six times). The time can be saved just in the beginning of the process, if we make faster initial dosage so that the reaction starts sooner. In the steady state, i.e. when temperature is close to the *370K*, higher dosage has minimal influence.

$\dot{m}_{FK}$ $[kg.s^{-1}]$	T_{max} [K]	T_{Vmax} [K]	a_{Fkmax} [-]	T_{total} [s]	T_{total} [h,m,s]
0,5	371,13	313,41	0,03535	25889	7, 11, 29
1	372,01	313,61	0,05279	25886	7, 11, 26
3	372,93	313,72	0,07623	25727	7, 8, 47

Table 2 Summary of values obtained by two step control with penalization

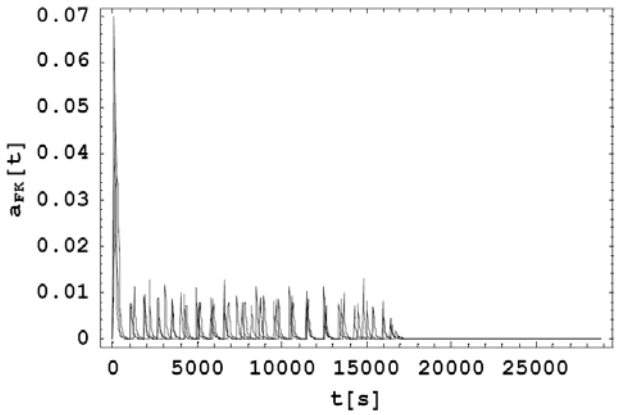

Fig. 10 The chromium sludge concentration development – two step control with penalization

The two step control with penalization provided these results (for the $F_1 = 3kg.s^{-1}$): the upper-most in-reactor temperature T reached 372.93 K, the maximum chromium sludge concentration a was 0.0762 and the total batch time made 25727 seconds. The in-reactor temperature oscillated around the desired value in the subrange of 7 Kelvin.

3.3 PID control

At first the unit step charakteristic identification using Strejc method was done [7]. On the model input was brought a step unit from 0 to 0.03 $kg.s^{-1}$. The obtained step response (figure 11) was modified to the unified form so that the steady state value equalled one's (figure 12). From the standardized form the delay time $T_{u,}$, rise time T_n and their proportion $\tau_u = T_u/T_n$ were determined. They had values: $T_{u,} = 180s$, $T_n = 11170s$, $\tau_u = 0.016$.

After that the approximation by the second order system was done. From the unified form (figure 12) was time t_1 determined; $y(t_1) = 0.720$, *i.e.* $t_1 = 10330s$. The t_1 is useful for the system time constants T_1 and T_2 determination:

$$T_1 + T_2 = \frac{t_1}{1.2564} \tag{6}$$

$\tau_u = T_u / T_n$	0,016	0,030	0,050	0,062	0,072
$\tau_2 = T_2 / T_1$	0,02	0,05	0,10	0,15	0,20
y_i	0,058	0,104	0,148	0,177	0,197
$\tau_u = T_u / T_n$	0,084	0,092	0,097	0,100	0,102
$\tau_2 = T_2 / T_1$	0,30	0,40	0,50	0,60	0,70
y_i	0,224	0,240	0,250	0,256	0,260
$\tau_u = T_u / T_n$	0,103	0,103	0,104		
$\tau_2 = T_2 / T_1$	0,80	0,90	1,00		
y_i	0,263	0,264	0,264		

Table 3 Time constants ratio τ_2 on the index point y_i and delay time to rise time ratio dependence

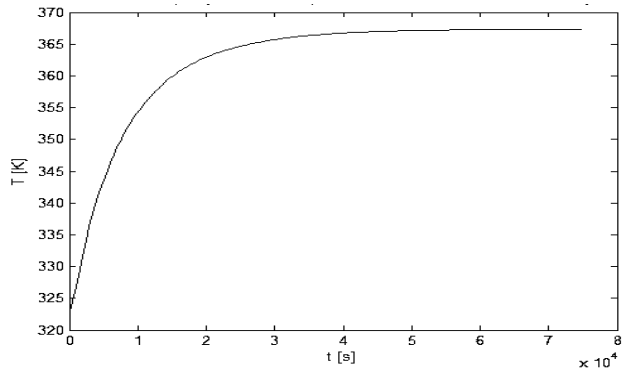

Fig. 11 Step response

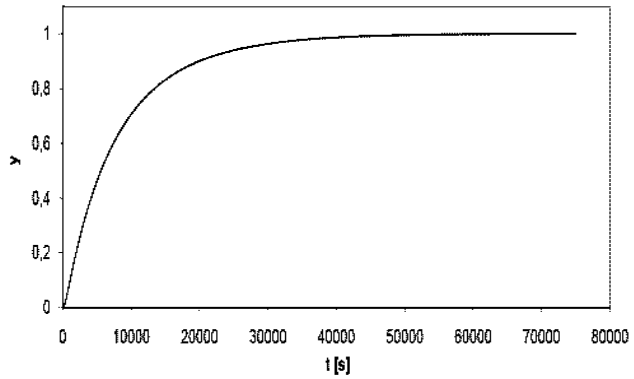

Fig. 12 Unified step response

With the help of the table 3 we can find the ratio of T_2/T_1 based on τ_u:

$$\frac{T_2}{T_1} = 0.02 \tag{7}$$

From equations 6 and 7 the $T_1 = 12725s$ and $T_2 = 254s$ values can be than counted. The gain constant K can be than obtained from the relation:

$$K = \frac{\Delta y}{\Delta u} = \frac{44.12}{0.03} = 1471 K / kg.s^{-1} \tag{8}$$

The final system transfer function has following form:

$$G(s) = \frac{1471}{(12725s + 1)(254s + 1)} \tag{9}$$

The final PID controller settings were: proportional part P = 0.033, integrative part I = 0.0000045 s, derivative part D = 1.2 s.

Diagrams with PID control results are displayed in figures 13, 14, 15, 16.

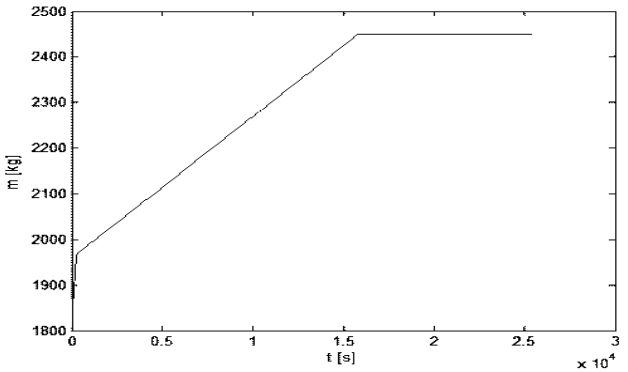

Fig. 13 The in-reactor mass development – PID control

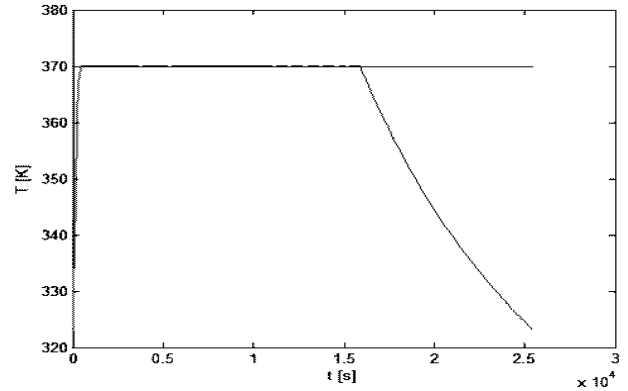

Fig. 14 The in-reactor temperature development – PID control

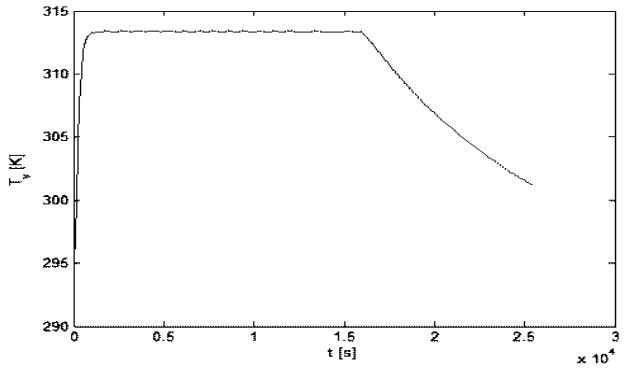

Fig. 15 The coolant temperature development – PID control

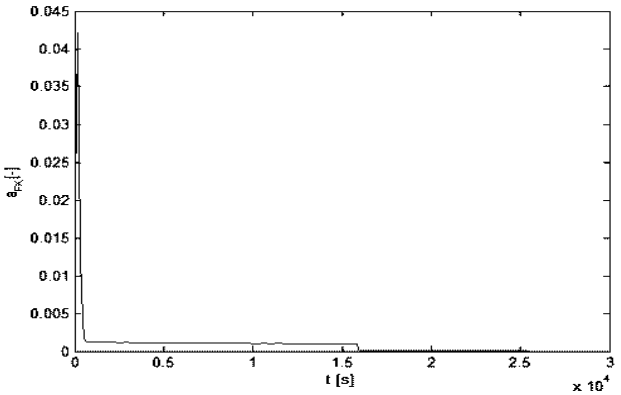

Fig. 16 The chromium sludge concentration development – PID control

The results of PID control were following: the upper-most in-reactor temperature T reached 370.22 K, the maximum chromium sludge concentration a was 0.0439 and the total batch time made 25491 seconds. The maximum and minimum actuating variable values were 1.546 kg.s^{-1} or 0 kg.s^{-1} respectively. The steady state actuating variable value made approximately 0.032 kg.s^{-1}.

3.4 Model predictive control

The basic idea of model predictive control (MPC) is to use a model to predict the future output trajectory of a process and compute a series of controller actions to minimize the difference between the predicted trajectory and a user-specified one, subject to constraints [8],[9].

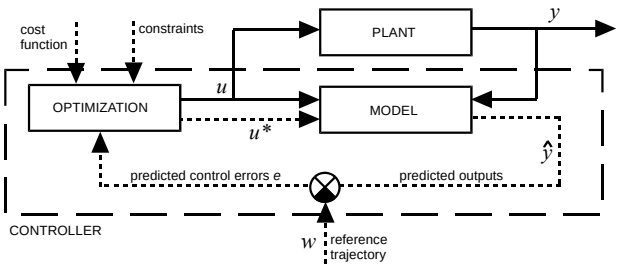

Fig. 17 The basic scheme of model predictive control

Generally we can say that MPC uses a predictor network (ANN) as the plant model in order to get its output predictions. The controller then calculates the control input that will optimize the performance criterion over a specified future time horizon [10]. Typical form of the performance criterion J is as follows:

$$J = \lambda \sum_{j=N_1}^{N_2} \left[y_r(k+j) - \hat{y}(k+j) \right]^2 +$$

$$+ \rho \sum_{j=1}^{N_u} \left[u_t(k+j-1) - u_t(k+j-2) \right]^2 \qquad (10)$$

where N_1, N_2 and N_u define horizons over which the tracking error and the control increments are evaluated. The u_t variable is the tentative control signal, y_r is the desired response and $\hat{y}$ is the predictor response. The λ and ρ parameters determine the contribution that the particular sum has on the performance index.

The selection of predictor is a key question in the model predictive control [11]. Because the controlled system is nonlinear, an artificial neural network (ANN) was selected [12]. After many simulations and tests the multilayered feed-forward neural network with three layers was chosen as the best solution from the wide group of artificial neural networks. From the figure 18 can be seen that as a transfer function the hyperbolic tangent was used in the both hidden layers, while in the output layer the linear function was applied. The ANN predictor used five last values of the system output and the controlled signal as an input. The ANN based predictor was trained offline using offline prepared identification data.

The minimization of the performance function is in the linear MPC typically provided by quadratic programming [13], [14]. Nevertheless, because of the nonlinearity of the predictor and the usage of constraints it was necessary to apply a numerical optimization method. Therefore, the Levenberg-Marquart method, which is implemented in the Matlab Optimization Toolbox [15], was used in this paper.

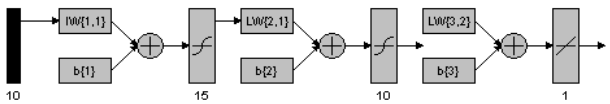

Fig. 18 The based on artificial neural network

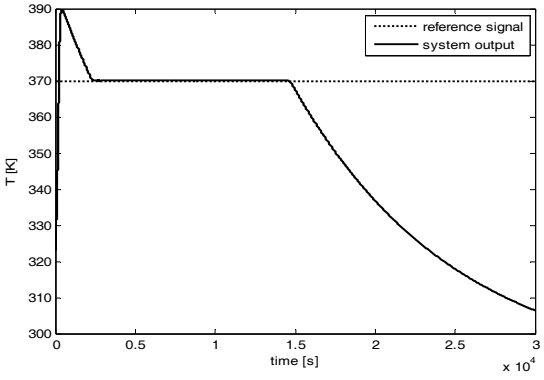

Fig. 19 The in-reactor temperature development – MPC1

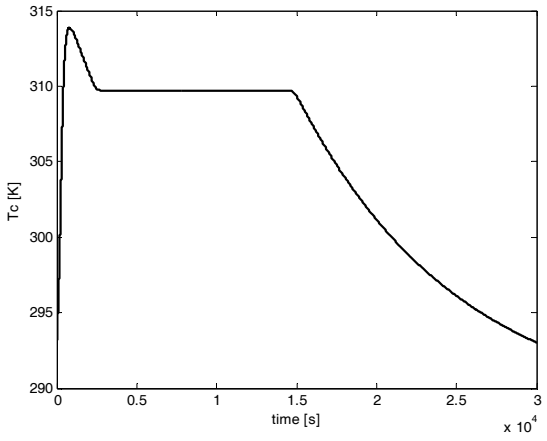

Fig. 20 The temperature in the cooling system – MPC1

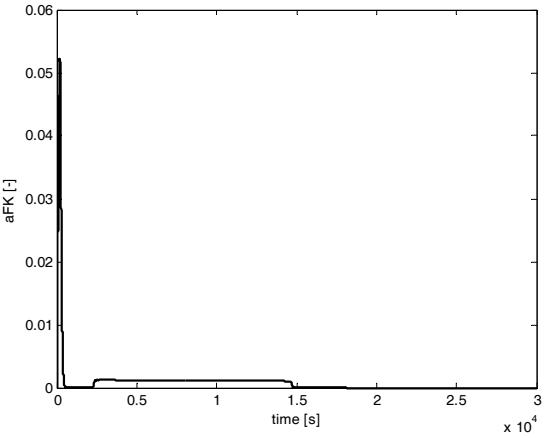

Fig. 21 The in-reactor chromium sludge concentration development – MPC1

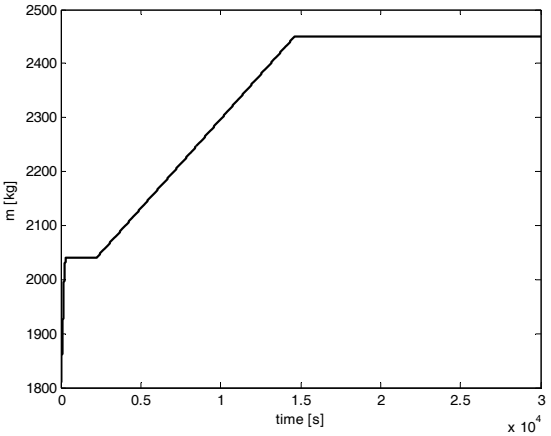

Fig. 22 The mass of reaction mixture – MPC1

In the figures 19, 20, 21 and 22 there are presented results of selected simulation of control using MPC controller with the criterion function (10). The presented simulation used the following settings of the controller: λ=1000, ρ =100000, N_1=1, N_2=8, N_u=8. However, this "standard" approach does not provide satisfactory performance in case of this semi-batch plant. The time of the batch must be as short as possible because of the economical reasons. But it is impossible to obtain fast batch without overshoot of temperature by any combination of controller parameters. The increase of ρ parameter can reduce the temperature overshoot but in the cost of long batch time.

Therefore, the third part to the criterion function (10) was added in order to reduce the speed of dosing (control signal u). The γ parameter determines the influence of nominal values of future control signal on the cost function (11). Results obtained using this cost function is in the following text denoted as MPC2. The settings of the controller were: λ=1000, ρ=10000, γ =10000, N_1=1, N_2=8, N_u=8. As can be seen from figures 23, 24, 25 and 26, the controller has permanent control error. In order to show this negative behaviour more clearly, it is assumed in the MPC2 that there is unlimited amount of the chromium sludge (batch input).

$$J = \lambda \sum_{j=N_1}^{N_2} \left[y_r(k+j) - \hat{y}(k+j) \right]^2 + \\ + \rho \sum_{j=1}^{N_u} \left[u_t(k+j-1) - u_t(k+j-2) \right]^2 + \\ + \gamma \sum_{j=1}^{Nu} u_t(k+j) \tag{11}$$

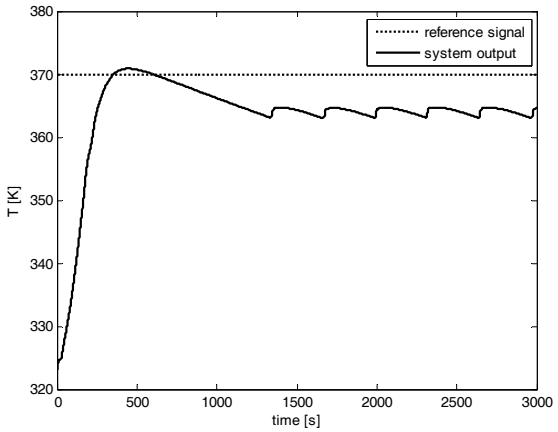

Fig. 23 The in-reactor temperature development – MPC2

It can be deduced from MPC2 results that the size of the control signal had to be penalized in the beginning of the batch only. Thus, the criterion function (11) was modified into the form defined by equations (12) and (13). Then, the γ parameter was during the control gradually decreased up to zero in

order to avoid the permanent control error. In other words, the third sum in the beginning of the control has the maximum value, and after initial phase it equals to zero. The γ_c parameter determines the speed of the decrement in γ.

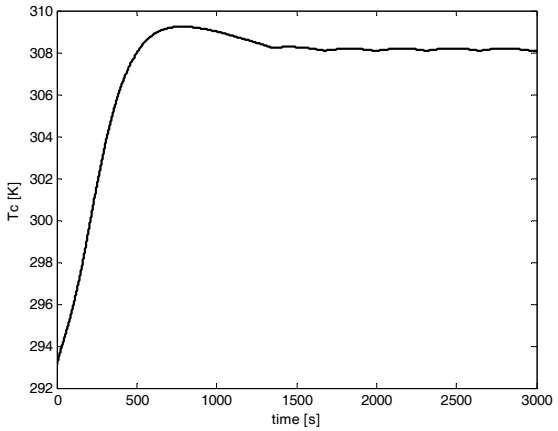

Fig. 24 The temperature in the cooling system – MPC2

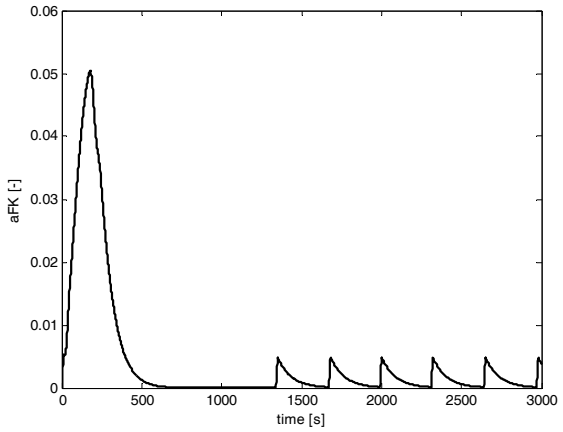

Fig. 25 The in-reactor chromium sludge concentration development – MPC2

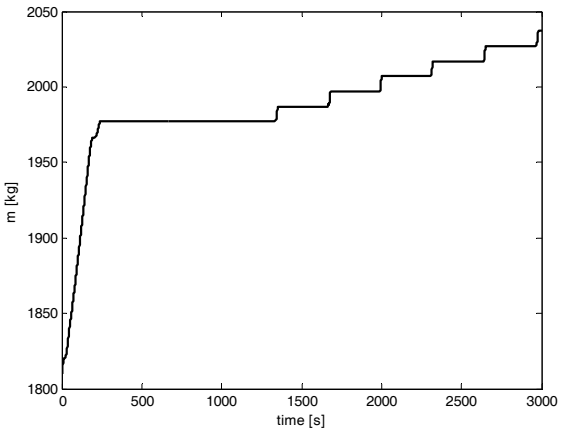

Fig. 26 The mass of reaction mixture – MPC2

$$J = \lambda \sum_{j=N_1}^{N_2} \left[y_r(k+j) - \hat{y}(k+j) \right]^2 + \\ + \rho \sum_{j=1}^{N_u} \left[u_t(k+j-1) - u_t(k+j-2) \right]^2 + \\ + \gamma(k) \sum_{j=1}^{N_u} u_t(k+j) \qquad (12)$$

$$\gamma(k) = \gamma(k-1) - \gamma_c \qquad (13)$$

The controller with cost function defined by equations (12) and (13) was tested in simulation MPC3 with the following settings: λ =1000, ρ =100000, γ=10000, γ_c =200, N_1=1, N_2=8, N_u=8. As can be seen from the figures 27 - 30, the MPC3 results were: the upper-most in-reactor temperature T reached 370.78 K, the maximum chromium sludge concentration a was 0.0461 and the total batch time made 25499 seconds.

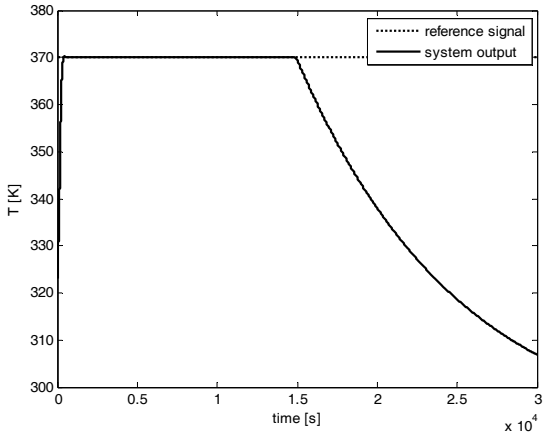

Fig. 27 The in-reactor temperature development – MPC3

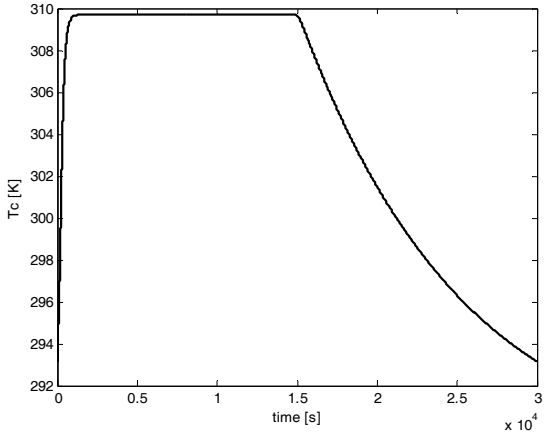

Fig. 28 The temperature in the cooling system – MPC3

The maximum and minimum actuating variable values were 0.9375 $kg.s^{-1}$ or 0 $kg.s^{-1}$ respectively. The steady state actuating variable value made approximately 0.031 $kg.s^{-1}$.

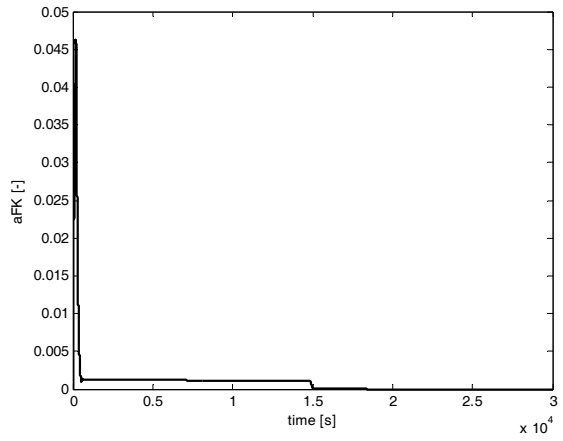

Fig. 29 The in-reactor chromium sludge concentration development – MPC3

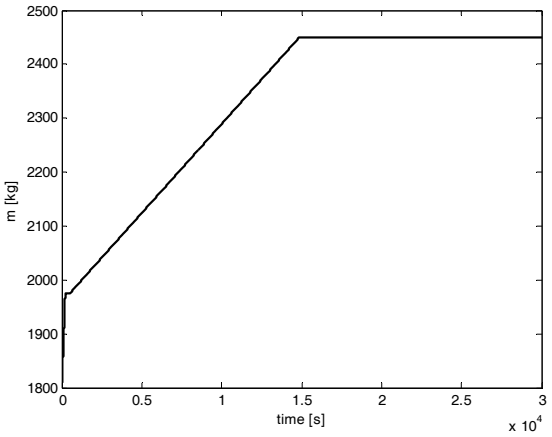

Fig. 30 The mass of reaction mixture – MPC3

4 Conclusion

It is difficult to distinguish which one of the shown control method was the best. The shortest process time provided the PID control method, but the difference with regard to MPC was only 8 seconds. The total process time took over 7 hours, so the difference 8 seconds can be neglected. The best control performance was obtained by MPC, but simulation of this method is quite hardware demanding today. The simulation using CPU 2500 MHz computer took almost 2 hours. The cheapest solution for an industrial application could be the two step control with penalization, but just in the case we don't need precise control performance.

5 Acknowledgement

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