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Predictive Control Using 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 sludge processing. 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. The control of the semi-batch reactor is difficult by common control methods because of the strongly exothermic chemical reaction. A model predictive control using artificial neural network is applied to the temperature control problem. The system control is generally complicated because of its nonlinearities.

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. One of the numerous possible solutions of the problem of chrome-tanned waste is its enzymatic dechromation. A chromium filter cake containing not only the alkali, but also a non-hydrolyzed protein is obtained. This fact can be used for the production of regenerated tanning chromium salts (Kolomazník at al. 2007).

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 (Hua at al. 2004).

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 (Bouhenchir at al. 2006): (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 model predictive control method application. The model input data comes from a real process - the chromium waste recycling process (Macků 2003), (Janáčová 2006). Let us consider single input – single output (SISO) system of chemical exothermic semi-batch reactor. The mathematical model of this system can be written by equations (1)-(4).

$$\frac{\mathrm{d}\,m(t)}{\mathrm{d}\,t} = F_I \tag{1}$$

$$\frac{\mathrm{d}\,a(t)}{\mathrm{d}\,t} = \frac{F_I}{m(t)} - A \cdot e^{-\frac{E}{R \cdot T(t)}} \cdot a(t) \tag{2}$$

$$\frac{\mathrm{d}\,T(t)}{\mathrm{d}\,t} = \frac{F_I \cdot c_I \cdot T_I}{m(t) \cdot c} + \frac{A \cdot e^{-\frac{E}{R \cdot T(t)}} \cdot \Delta H_r \cdot a(t)}{c} - \frac{K \cdot S \cdot T(t)}{m(t) \cdot c} + \frac{K \cdot S \cdot T_C(t)}{m(t) \cdot c} \tag{3}$$

$$\frac{\mathrm{d}T_C(t)}{\mathrm{d}t} = \frac{F_C \cdot T_{CI}}{m_C} + \frac{K \cdot S \cdot T(t)}{m_C \cdot c_C} - \frac{K \cdot S \cdot T_C(t)}{m_C \cdot c_C} - \frac{F_C \cdot T_C(t)}{m_C} \quad (4)$$

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 = 29967.509 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.

3. MODEL PREDICTIVE CONTROL

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}.

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 (Garcia at al. 1989), (Camacho 2004), Fig. 1.

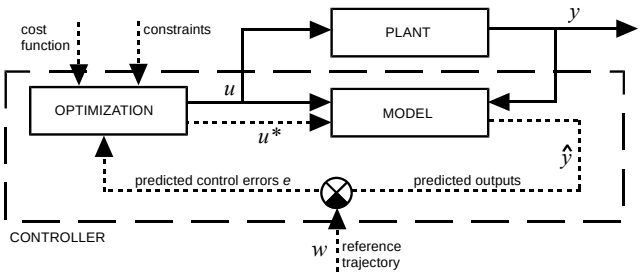

Fig. 1. The basic scheme of model predictive control.

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 (Zhang 2008). Typical form of the performance criterion J is as follows:

$$J = \lambda \sum_{j=N_1}^{N_2} \left[y_r(k+j) - \hat{y}(k+j) \right]^2 + \rho \sum_{j=1}^{N_u} \left[u_t(k+j-1) - u_t(k+j-2) \right]^2 \quad (5)$$

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 (Mazinan 2008). Because the controlled system is nonlinear, an artificial neural network (ANN) was selected (Volosencu 2009). 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 2 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 (Tondel at al. 2003), (Kouvaritakis at al. 2002). 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 (Venkataraman 2009), was used in this paper.

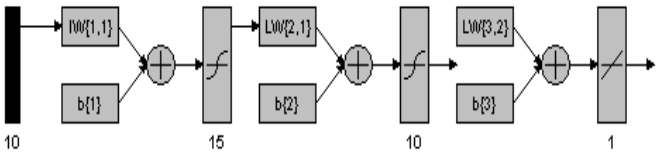

Fig. 2. The based on artificial neural network.

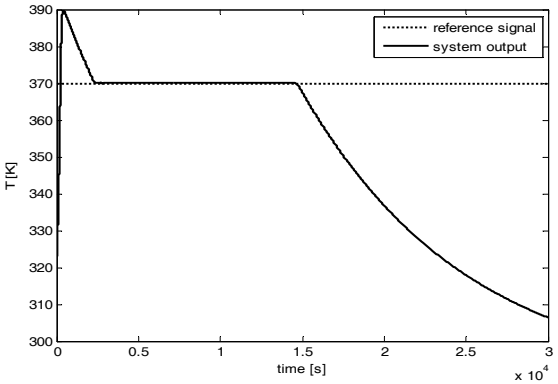

Fig. 3. The in-reactor temperature development – MPC1.

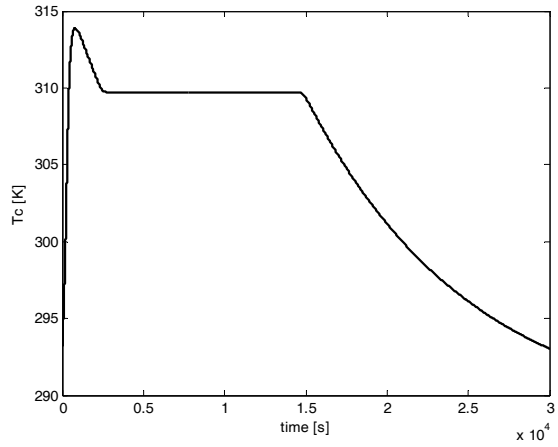

Fig. 4. The temperature in the cooling system – MPC1.

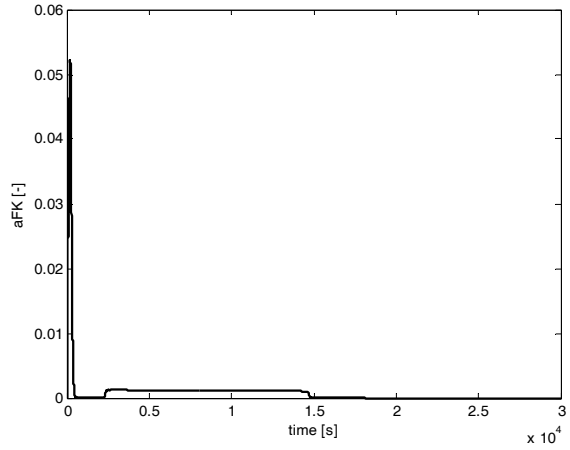

Fig. 5. The in-reactor chromium sludge concentration development – MPC1.

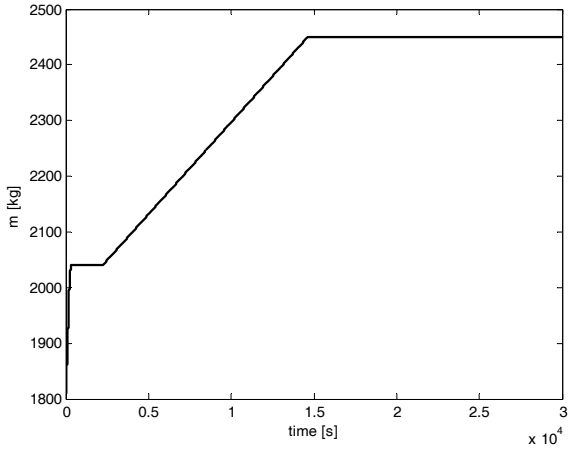

Fig. 6 The mass of reaction mixture – MPC1.

In the figures 3, 4, 5 and 6 there are presented results of selected simulation of control using MPC controller with the criterion function (6). 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 (5) was added in order to reduce the speed of dosing (control signal $\underline{u}$). The γ parameter determines the influence of nominal values of future control signal on the cost function (6). 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 7, 8, 9 and 10, 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).

$$J = \lambda \sum_{j=N_1}^{N_2} \left[y_r(k+j) - \hat{y}(k+j) \right]^2 + \rho \sum_{j=1}^{N_u} \left[u_t(k+j-1) - u_t(k+j-2) \right]^2 + \gamma \sum_{j=1}^{Nu} u_t(k+j) \quad (6)$$

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 (6) was modified into the form defined by equations (7) and (8). 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.

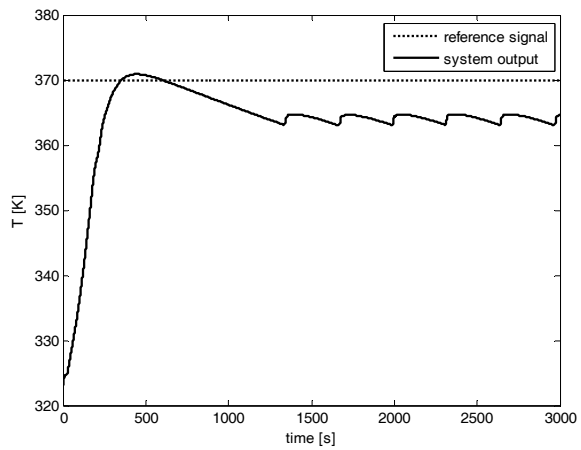

Fig.7 The in-reactor temperature development – MPC2.

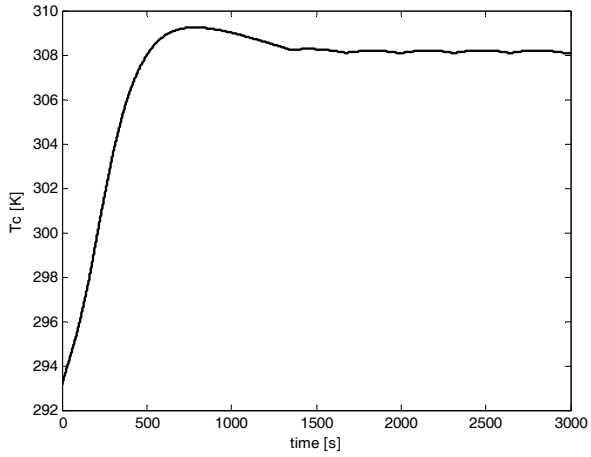

Fig.8 The temperature in the cooling system – MPC2.

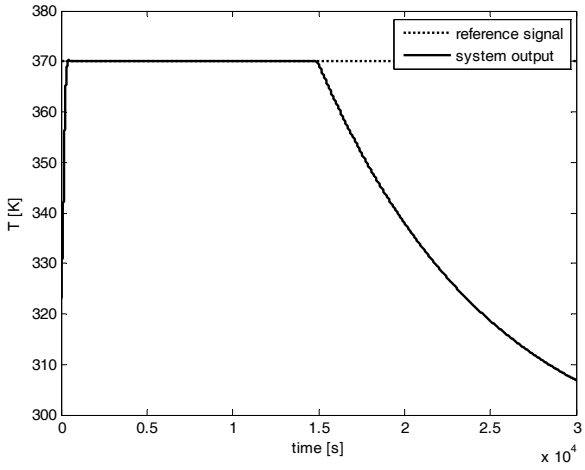

Fig.11 The in-reactor temperature development – MPC3.

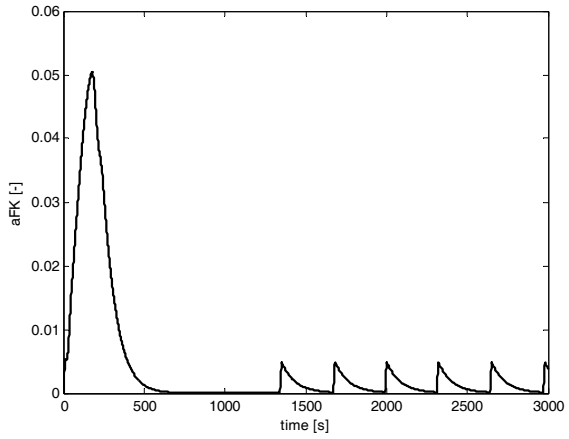

Fig.9 The in-reactor chromium sludge concentration development – MPC2.

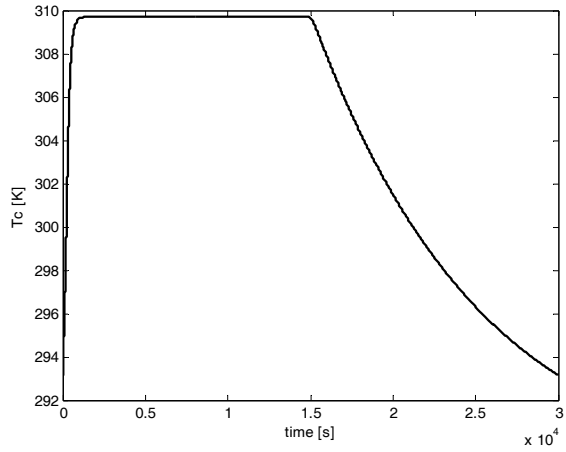

Fig.12 The temperature in the cooling system – MPC3.

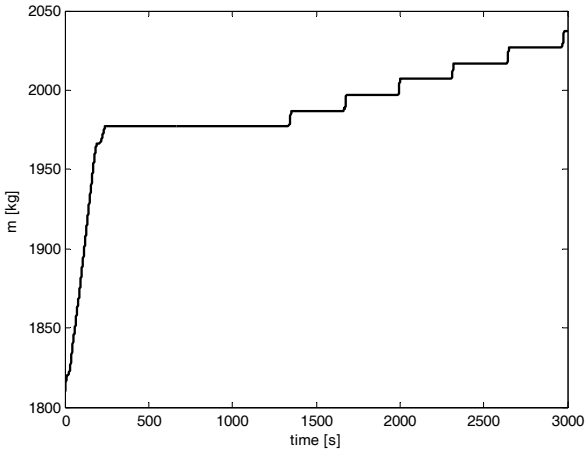

Fig.10 The mass of reaction mixture – MPC2.

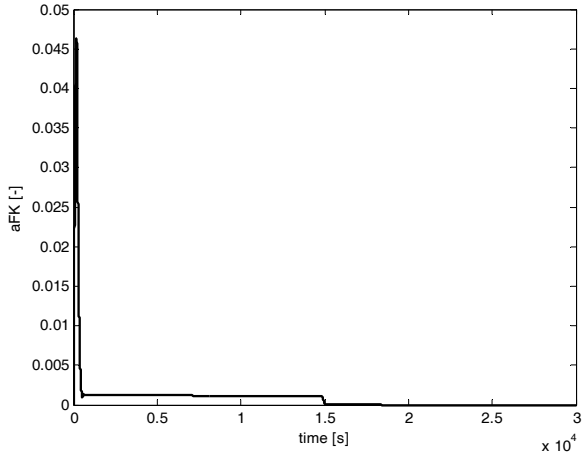

Fig.13 The in-reactor chromium sludge concentration development – MPC3.

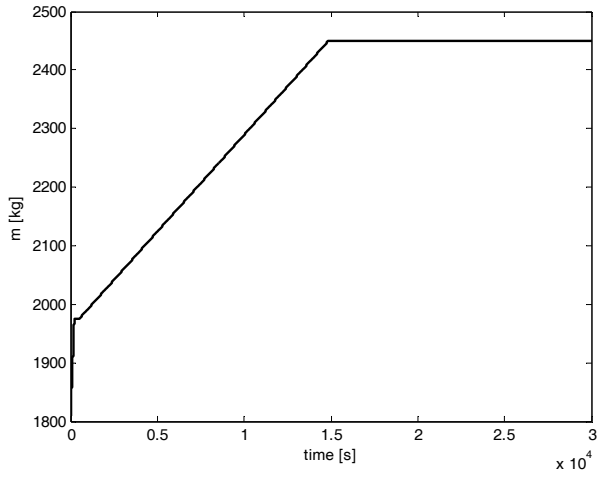

Fig.14 The mass of reaction mixture – MPC3.

$$J = \lambda \sum_{j=N_1}^{N_2} \left[y_r(k+j) - \hat{y}(k+j) \right]^2 + \rho \sum_{j=1}^{N_u} \left[u_t(k+j-1) - u_t(k+j-2) \right]^2 \quad (7)$$

$$\gamma(k) \sum_{j=1}^{N_u} u_t(k+j)$$

$$\gamma(k) = \gamma(k-1) - \gamma_c \quad (8)$$

The controller with cost function defined by equations (7) and (8) 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 11 – 14, 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.

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.

4. CONCLUSION

The best control performance was obtained by MPC3, but simulation of this method is quite hardware demanding today. The simulation using CPU 2500 MHz computer took almost 2 hours. As can be seen, the MPC can solve even such difficult task as nonlinear system, chemical reactor is.

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