SIMULATION OF MODEL PREDICTIVE CONTROL OF SEMI-BATCH REACTOR

David Samek*, Lubomir Macku**

*Tomas Bata University in Zlin, Faculty of Technology, Department of Production Engineering
**Tomas Bata University in Zlin, Faculty of Applied Informatics, Department of Electrotechnics and Measurements

Abstract: The aim of this paper is to present simulation of model predictive control of chemical exothermic semi-batch reactor model, while the MPC controller uses an artificial neural network as a predictor. A first order chemical reaction is considered to be running in the reactor. The reaction is strongly exothermic so the in-reactor temperature is rising very fast due to reaction component dosing. Thus, the temperature control is necessary. The system is nonlinear because of chemical reaction kinetics, so its control is difficult by classical methods.

Keywords: modelling, simulation, artificial neural networks, model predictive control, batch reactor.

1. INTRODUCTION

Batch processing is widely used in the chemical industry. A wide range of various chemicals, dyes, composites, polymers, cosmetic, pharmaceutical, food and agricultural products are produced in batch operations (Srinivasan and Bonvin, 2007). In this paper the temperature in the chemical exothermic semi-batch reactor is controlled. The considered reactor is used for the chromium waste recycling process based on the enzymatic hydrolysis (Kolomaznik et al., 1996). The chromium waste comes from 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; it is a waste free technology. The reactor deals with a problem of chromium sludge (chromium filter cake) reusing.

The control of this reactor is very difficult because the temperature is rising very quickly with very small amount of added reactant (Macku, 2005).

One of the successful control techniques for batch and semi-batch processing control is Model predictive control (MPC) (Richards and Congalidis, 2006), whereas this method is adopted in the paper. Because of the system complexity and nonlinearity the artificial neural network (ANN) is used as a black-box model which predicts the system outputs.

The contribution is organized as follows: the semi-batch reactor is described in the next chapter. Then the model predictive control using artificial neural networks is introduced. The following chapter provides description of simulations, their results and discussions. The paper is concluded by final remarks in the chapter 5.

2. DESCRIPTION OF THE CHEMICAL SEMI-BATCH REACTOR

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:

$$2C_{6}H_{8}NO + 5K_{2}Cr_{2}O_{7} + Cr_{2}O_{3} + 23H_{2}SO_{4} \rightarrow 6CO_{2} + N_{2} + 28H_{2}O + 5K_{2}SO_{4} + 6Cr_{2}(SO_{4})_{3}$$  \hspace{1cm} (1)

where $C_{6}H_{8}NO$ is the protein and $Cr_{2}O_{3}$ is the chromium trioxide that are main compounds of the chromium sludge. The sulphuric acid ($H_{2}SO_{4(aq)}$) and the potassium dichromate ($K_{2}Cr_{2}O_{7(aq)}$) 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.

$$\frac{dT(t)}{dt} = \frac{F_{I} \cdot c_{I} \cdot T_{I}}{m(t) \cdot c} + \frac{A \cdot e^{-\frac{E}{RT(t)}} \cdot \Delta H_{r} \cdot a(t)}{c} - \frac{K \cdot S \cdot T(t)}{m(t) \cdot c} + \frac{K \cdot S \cdot T_{c}(t)}{m_{c} \cdot c_{c}}$$  \hspace{1cm} (4)

$$\frac{dT_{c}(t)}{dt} = \frac{F_{c} \cdot T_{cI}}{m_{c}} + \frac{K \cdot S \cdot T(t)}{m_{c} \cdot c_{c}} - \frac{K \cdot S \cdot T_{c}(t)}{m_{c} \cdot c_{c}}$$  \hspace{1cm} (5)

where $m$ is the total weight of reaction components in the reactor, $a$ is the mass concentration of the chromium sludge in the chemical 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 chromium sludge input mass flow rate, temperature and specific heat capacity, respectively, $F_{c} = 1$ 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$^{-1}$, $\Delta H_{r} = 1392350$ J·kg$^{-1}$, $K = 200$ kg·s$^{-3}$·K$^{-1}$, $S = 7.36$ m$^{2}$.

Fig. 1. Exothermic chemical semi-batch reactor.

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).

$$\frac{dm(t)}{dt} = F_{I}$$  \hspace{1cm} (2)

$$\frac{da(t)}{dt} = \frac{F_{I}}{m(t)} - A \cdot e^{-\frac{E}{RT(t)}} \cdot a(t)$$  \hspace{1cm} (3)

Theoretically, the temperature in the reactor $T$ could be driven by manipulating input temperature $T_{cI}$ and mass flow rate of cooling water $F_{c}$ and mass flow rate of the chromium sludge $F_{I}$. However, after the economical analysis there was decided to control the temperature by manipulating the flow rate of the chromium sludge only. It is due to the strong exothermic nature of the reaction (the temperature rises very quickly with very small concentration of the chromium sludge $a$). Thus, it is cheaper to set the flow of the cooling water to the maximal reasonable value ($F_{c} = 1$ kg·s$^{-1}$) and use readily available water with average temperature $T_{cI} = 288.15$ K = 15 °C for cooling. In other words, the task of the controller is...
to control the temperature $T$ by manipulating the control signal $F_t$.

The chemical reaction described by the equation (1) runs the faster the higher the temperature is. Nevertheless, the reaction mixture contains a lot of water and it is necessary to keep the water in the liquid state. Therefore, the desired value of the $T$ is 370 K, but the maximum acceptable temperature is 373 K. The maximum flow rate of the mud pump, which is used for the chromium sludge dosing, is 3 kg·s$^{-1}$, hence the control signal has to be in the interval $<0, 3>$ kg·s$^{-1}$.

3. MODEL PREDICTIVE CONTROL USING ARTIFICIAL NEURAL NETWORK

This chapter is divided into two parts. The first part is devoted to Model predictive control method, while the second part describes application of artificial neural network as the predictor in the MPC controller.

3.1 Model predictive control

The basic idea of 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 et al., 1989). Generally we can say that MPC use 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. Typical form of the performance criterion $J$ is as follows (Kanjilal, 1995):

$$J = \lambda \sum_{j=N_1}^{N_2} [y_j(k+j) - \hat{y}(k+j)]^2 +$$
$$+ \rho \sum_{j=1}^{N_3} [u_{j}(k+j-1) - u_{j}(k+j-2)]^2$$

(6)

where $N_1$, $N_2$ and $N_3$ define horizons over which the tracking error and the control increments are evaluated. The $u_j$ variable is the tentative control signal, $y_j$ is the desired response and $\hat{y}$ is the predictor response. The $\lambda$ and $\rho$ parameters determine the contribution that the particular sum has on the performance index.

Due to the particular plant behaviour, the size of the control signal had to be penalized in the beginning of the batch. Thus, in this paper the third part of the criterion was added while the $\gamma$ parameter determines the contribution that the third sum has on the performance index. Because the control signal is constrained to the interval $<0, 3>$ kg·s$^{-1}$, it wasn’t necessary to use absolute values or squares in the third sum. However, in order to avoid the permanent control error the $\gamma$ parameter was during the control gradually decreased up to zero. In other words, the third part of the criterion has the maximum value in the beginning of the control, and after initial phase it equals to zero.

$$J = \lambda \sum_{j=N_1}^{N_2} [y_j(k+j) - \hat{y}(k+j)]^2 +$$
$$+ \rho \sum_{j=1}^{N_3} [u_{j}(k+j-1) - u_{j}(k+j-2)]^2 +$$
$$+ \gamma(k) \sum_{j=1}^{N_3} u_{j}(k+j)$$

(7)

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

(8)

where $\gamma_c$ is the parameter which defines the speed of the decrement in $\gamma$.

Model predictive controllers can generally use various predictors. The predictors can be divided into two main groups (Smith, 2003): white box models and black box models. The white box modelling is established on a prior knowledge of mathematic description of basic physical rules of controlled process. White box models are excellent for process modelling and product development. The model constants have a physical meaning and are not dependent on process design. The main disadvantage of white box models is the time of development and higher complexity. Conversely, black box models such as artificial neural network (ANN) and fuzzy logic models are data-driven. They provide general method for process dynamics description from input-output data. First and foremost, the learning ability makes artificial neural networks versatile, user friendly and powerful tool for many practical applications (Hussain, 1999).

3.2 Artificial neural networks

There are many types of artificial neural networks which are suitable for modelling and prediction of either linear or nonlinear systems. The most popular type of ANNs in the MPC is the multilayer feed-forward neural network (MFFNN) (Hagan et al., 2002), which is adopted in this paper.

In the MFFNN the signals flow between the neurones only in the forward direction i.e. towards the output. Neurons of the layer can have inputs from any neurones of the earlier layer. Each neurone is characterized by the generally nonlinear transfer function $S$ and by the threshold value $b$. The neurone sums the weighted inputs and the threshold, and passes the result through its characteristic transfer function. The transfer function is usually same for all neurones from the layer.

Weights are commonly labelled $w_{\text{number of layers}}$ thresholds likewise. Values can be arranged into
matrixes and the function of the three-layered feed-forward neural network can be written:

\[ y_{\text{out}} = S_i(b_i + W_i \cdot x_i) \]  \hspace{1cm} (9) \\
\[ x_2 = S_2(b_2 + W_2 \cdot x_1) \]  \hspace{1cm} (10) \\
\[ x_1 = S_1(b_1 + W_1 \cdot u) \]  \hspace{1cm} (11)

where \( y_{\text{out}} \) is output vector, \( u \) is input vector, \( S_i \) is transfer function of the \( i \)-th layer, \( b_i \) is threshold vector of the \( i \)-th layer, \( W_i \) is weight matrix of \( i \)-th layer and \( x_i \) is output vector from \( i \)-th layer.

4. SIMULATIONS AND RESULTS

All simulations were done in Matlab/Simulink. Model of the reactor was programmed as the S-Function, while the MPC controller as the M-Function. The sampling time in all simulations was set to 10 s.

The predictor based on MFFNN had three layers that can be described by the equations (9)-(11). Both hidden layers contained neurons with hyperbolic tangent transfer function, while the output layer contained neurons with linear transfer function. The simplified scheme of the artificial neural network is depicted in the figure 3. The predictor was trained off-line.

![Simplified scheme of the predictor based on MFFNN.](image)

The minimization of the performance function is in the linear MPC typically provided by quadratic programming. 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, was used in this paper.

As was mentioned thereinbefore, the chemical reaction is strongly exothermic and usage of the cost function in the classical form (6) is unsuitable. The results obtained using this cost function are presented in the figures 4-7. The setting of the reactor: \( \lambda = 1000, \rho = 100000, N_1 = 1, N_2 = N_3 = 8 \). This simulation is in the following text denoted as sim1.

The dosing finishes at the time of 14649s (4h 4min 9s), because the whole amount of the chromium sludge is consumed. Then the manipulating variable equals to zero, the controller is switched off and the reactor is only cooled by the double wall cooling system. The batch is completed when the temperature of the reaction mixture reaches discharge value. As can be seen from the figures, the temperature of the reaction mixture exceeded the maximum limit of 373 K. This behaviour is caused by very steep rise of the chromium sludge concentration in the reactor. This effect could be suppressed by slower dosing of the chromium sludge, which can be achieved by increasing the \( \rho \) parameter. However, this would lead to prolongation of the batch time, which is economically unprofitable.

![The course of the controlled variable \( y \) (temperature of reaction mixture \( T \)), desired value \( y_r \) and output temperature of cooling water \( T_C \) in the simulation sim1.](image)

![The course of the manipulated variable \( u \) (mass flow rate of the chromium sludge \( F_I \)) in the simulation sim1.](image)

![The course of the reaction mixture mass \( m \) in the simulation sim1.](image)
To cope with the temperature overshoot the penalization of the nominal value of the manipulating variable was added to the cost function (eq. 7, 8). This simulation is in the following text denoted as the \textit{sim2}. As was mentioned thereinbefore, the manipulating variable is penalized only in the beginning of the batch. The parameters $\gamma$ and $\gamma_c$ were set to 10000 and 200, respectively. Thus, the third part in the equation 7 equals to zero from the time of 500s (the 50\textsuperscript{th} step). The rest of the parameters remain the same as in the \textit{sim1}. The results of simulation \textit{sim2} are presented in the figures 8-11. As can be seen from the figures the overshoot doesn’t exceed the limit of 373K. The penalization of the manipulating variable slows down the increase of the chromium sludge concentration $a$ and consequently the increase of the reaction mixture temperature $T$. The time of the dosing is 14880s (4h 8min). However, there is still a small overshoot of the controlled variable (see Table 1).

This overshoot can be reduced by increasing the $\gamma$ parameter. In the simulation \textit{sim3} was parameter $\gamma$ set to 15000, the rest of the parameters remains the same as in the \textit{sim2}. The results of the simulation \textit{sim3} are demonstrated in the figures 12-15.

To compare the simulations let us to define $y_{\text{max}}$ as a maximal overshoot, $t_0$ as the time of the reaction (dosing), number of steps $t_f = 1400$ (= 14000s) and criterions $S_u$ and $S_y$:

$$S_u = \sum_{i=0}^{t_f} (u(i+1) - u(i))^2$$  \hspace{1cm} (12)

$$S_y = \sum_{i=0}^{t_f} (y_Y(i) - y(i))^2$$  \hspace{1cm} (13)

<table>
<thead>
<tr>
<th>$y_{\text{max}}$</th>
<th>$S_u$ ($\text{Kg}^2\cdot\text{s}^2$)</th>
<th>$S_y$ ($\text{K}^2$)</th>
<th>$t_0$ ($\text{s}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>\textit{sim1}</td>
<td>389.9</td>
<td>6.56</td>
<td>4.9 \times 10^5</td>
</tr>
<tr>
<td>\textit{sim2}</td>
<td>370.3</td>
<td>1.06</td>
<td>2.5 \times 10^5</td>
</tr>
<tr>
<td>\textit{sim3}</td>
<td>370.2</td>
<td>0.47</td>
<td>2.4 \times 10^5</td>
</tr>
</tbody>
</table>

\textbf{Table 1} Comparison of the the simulations

Fig. 7. The course of the mass concentration of the chromium sludge in the chemical reactor $a$ in the simulation \textit{sim1}.

Fig. 8. The course of the controlled variable $y$ (temperature of reaction mixture $T$), desired value $y_r$ and output temperature of cooling water $T_C$ in the simulation \textit{sim2}.

Fig. 9. The course of the manipulated variable $u$ (mass flow rate of the chromium sludge $F_I$) in the simulation \textit{sim2}.

Fig. 10. The course of the reaction mixture mass $m$ in the simulation \textit{sim2}.

Fig. 11. The course of the mass concentration of the chromium sludge in the chemical reactor $a$ in the simulation \textit{sim2}.
5. CONCLUSION

This paper dealt with the study of the MPC control of the nonlinear chemical exothermic semi-batch reactor. Artificial neural network was chosen as the predictor due to the nonlinearity of the plant. The typical form of the MPC cost function had been modified in order to cope with the overshoots of controlled temperature.

As can be seen from the presented figures and the table the enhancement of the cost function provides significantly better results from the point of view of control error and overshoot at the cost of minor time prolongation and slightly oscillating course of controlled variable.

ACKNOWLEDGEMENT

This work was supported by the Grant Agency of the Czech Republic under grant 102/07/P137 and by the Ministry of Education, Youth and Sports of the Czech Republic under grant MSM 7088352102. This support is gratefully acknowledged.

REFERENCES


