Optimal operating strategies for semi-batch reactor used for chromium sludge regeneration process

NOVOSAD DAVID, MACKŮ LUBOMÍR
Tomas Bata University in Zlin
Faculty of Applied Informatics
nám. T.G.Masaryka 5555, 760 05 Zlín
CZECH REPUBLIC
novosad@fhs.utb.cz http://www.fai.utb.cz

Abstract: - This paper deals with controlling of a semi-batch nonlinear reactor used for chromium sludge regeneration process. The aim is to process the largest amount of chromium filter cake (chromium sludge) in the shortest possible time. The reactor has to be cooled because of strongly exothermic process. For safety reasons the temperature should not exceed 100 °C. In this study the reactor is controlled by two manipulating inputs: filter cake feeding flow rate and cooling water temperature. The speed of the whole process depends on the filter cake feeding flow rate – in case of a large amount filter cake addition a sharp temperature rise follows. The controller must be able to find optimal strategy between the filter cake dosing and the cooling temperature to reach the shortest possible process time. In order to deal with process nonlinearities here an online identification must be used. Results obtained using the proposed control method are then compared with our previous research, especially with control method using only one manipulating input - filter cake feeding flow rate.

Key-Words: temperature control; online identification; semi-batch reactor; PID; pole placement

1 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.

The temperature profile during the recycling operation 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.

In the literature some papers have been published which discuss the control of a batch or semi-batch reactor. For example Beyer et al. applied a global linearization control strategy with online state and parameter estimation for a polymerization reactor [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 study [4], where the authors applied a dual-mode (DM) 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 [5] was recommended. 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 for identification and control time-varying-delayed nonlinear dynamic systems. Neural networks are often presented as a good method to reach useful results in batch processes. An appropriate selection of the manipulated variable is necessary to selecting the proper control strategy. In a recent article dealing with production of ethyl acrylate in CSTR, five different pairs of manipulated variables were compared [7]. The final recommended control...
strategy contained two manipulated variables – feeding flow rates of both reactants. This newly proposed method showed better results than the previously used strategy with only one manipulated variable. Similarly, in our article we will focus on the use of two manipulated variables instead of one.

This paper presents results of experiments obtained by real process simulations. These simulations involved the control of the semi-batch process using PID controller tuned using pole placement method (PIDPP). This method using only one manipulated variable was tested in our previous works [8] and is now extended to control two manipulated variables simultaneously. The whole process is supposed to run in the reactor located in Kortan company in Hrádek nad Nisou [9]. Because of that fact the mathematical model was designed for this reactor, which dimensions and geometry are shown in the Fig. 1.

Figure 1. Exothermic chemical semi-batch reactor

The paper is organized as follows. In section II, the semi-batch reactor and structure of the controller are described; section III presents simulation results and section IV concludes the current work and suggests new areas for investigation.

2 Methods section

2.1 The semi-batch reactor model

To simulate tanning salts from the chromium sludge regeneration process a mathematical model is used. The reactor has four input signals \( \dot{m}_{FK}(t) \), \( m_{FP}(t) \), \( T_{FK}(t) \), \( T_{FP}(t) \) and one output signal \( T(t) \) [10]. The chemical reactor scheme is shown in Fig. 2.

![Figure 2. Chemical reactor scheme](image)

Implementation of the method and all simulations are done in MATLAB/Simulink software. The mathematical model of the fed-batch reactor is defined by differential Eq. (1-4).

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

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

\[
\dot{m}_{FK}c_{FK}T_{FK} + \Delta H c_{FK}k m(t) a_{FK}(t) = K S [T(t) - T_{r}(t)] + \frac{d}{dt} [m(t)c_{FK}T(t)] \tag{3}
\]

\[
\dot{m}_{FP}c_{FP}T_{FP} + K S [T(t) - T_{r}(t)] = \dot{m}_{FP}c_{FP}T_{FP}(t) + m_{FP}c_{FP}T_{FP} \tag{4}
\]

The first equation expresses the total mass balance of the chemical solution in the reactor. The symbol \( \dot{m}_{FK} \) [kg/s] expresses the mass flow of entering chromium sludge, \( \frac{d}{dt} m(t) \) the accumulation of the in-reactor content.

The second equation expresses the chromium sludge mass balance. The input is \( m_{FK} \) [kg/s] again, the accumulation is \( m(t) \) and the express \( k m(t)a_{FK}(t) \) means the chromium sludge extinction by the chemical reaction. Symbol \( k \) [s^{-1}] means...
The reaction rate constant expressed by an Arrhenius equation (5).

\[ k = A e^{-\frac{E}{RT(t)}} \]  

(5)

Knowledge of the Arrhenius equation parameters leads to the correct mathematical model, which is linked with safe and successful control [11]. Variables and parameters of the reactor are given in Table 1.

Table 1 - Variables and parameters of the reactor model

<table>
<thead>
<tr>
<th>Description</th>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow of the entering chromium sludge</td>
<td>( \dot{m}_{FK} )</td>
<td>[kg.s(^{-1})]</td>
</tr>
<tr>
<td>Accumulation of the in-reactor content</td>
<td>( m(t) )</td>
<td>[kg]</td>
</tr>
<tr>
<td>Mass concentration of the chromium sludge</td>
<td>( a_{FK}(t) )</td>
<td>[-]</td>
</tr>
<tr>
<td>Weight of the reaction components in the system</td>
<td>( m(t) )</td>
<td>[kg]</td>
</tr>
<tr>
<td>Reaction rate constant</td>
<td>( k )</td>
<td>[s(^{-1})]</td>
</tr>
<tr>
<td>Chromium sludge specific heat capacity</td>
<td>( c_{FK} )</td>
<td>[J.kg(^{-1}).K(^{-1})]</td>
</tr>
<tr>
<td>Reactor content specific heat capacity</td>
<td>( c_p )</td>
<td>[J.kg(^{-1}).K(^{-1})]</td>
</tr>
<tr>
<td>Chromium sludge temperature</td>
<td>( T_{FK} )</td>
<td>[K]</td>
</tr>
<tr>
<td>Reaction heat</td>
<td>( \Delta H_r )</td>
<td>[J.kg(^{-1})]</td>
</tr>
<tr>
<td>Conduction coefficient</td>
<td>( K )</td>
<td>[J.m(^{-2}).K(^{-1}).s(^{-1})]</td>
</tr>
<tr>
<td>Heat transfer surface</td>
<td>( S )</td>
<td>[m(^2)]</td>
</tr>
<tr>
<td>Temperature of reaction components in the reactor</td>
<td>( T_r(t) )</td>
<td>[K]</td>
</tr>
<tr>
<td>Temperature of coolant in the reactor double wall</td>
<td>( T_c(t) )</td>
<td>[K]</td>
</tr>
<tr>
<td>Coolant mass flow</td>
<td>( \dot{m}_c )</td>
<td>[kg.s(^{-1})]</td>
</tr>
<tr>
<td>Coolant specific heat capacity</td>
<td>( c_c )</td>
<td>[J.kg(^{-1}).K(^{-1})]</td>
</tr>
<tr>
<td>Input coolant temperature</td>
<td>( T_{ip} )</td>
<td>[K]</td>
</tr>
<tr>
<td>Coolant mass weight in the reactor double wall</td>
<td>( m_c )</td>
<td>[kg]</td>
</tr>
<tr>
<td>Pre-exponential factor</td>
<td>( A )</td>
<td>[s(^{-1})]</td>
</tr>
<tr>
<td>Activation energy</td>
<td>( E )</td>
<td>[J.mol(^{-1})]</td>
</tr>
<tr>
<td>Gas constant</td>
<td>( R )</td>
<td>[J.mol(^{-1}).K(^{-1})]</td>
</tr>
</tbody>
</table>

\( a_{FK}(t) \) means mass fraction of chromium sludge in the chemical reactor, \( m(t) \) weight of reaction components in the reactor.

The third equation describes enthalpy balance. The reactor input heat is expressed by \( \dot{m}_{FK} c_{FK} T_{FK} \), the heat rising from the chemical reaction is \( \Delta H_r k m(t) a_{FK}(t) \), the reactor wall heat transmission is \( K S (T_r(t) - T_{ip}(t)) \) and the accumulated heat inside the reactor is described by \( m(t) c_r \frac{d}{dt} T(t) \). The last equation describes a coolant balance. The coolant input heat is expressed by, \( \dot{m}_c c_c T_{ip} \) the heat entering to the coolant from the reactor by the reactor wall is, \( K S (T_r(t) - T_{ip}(t)) \) the heat going out with the coolant is \( \dot{m}_c c_c T_{ip}(t) \) and the heat accumulated in the double wall coolant expresses \( m_{FK} c_c \frac{d}{dt} T_{ip}(t) \). Detailed description of this model is given in [12]. This model model cannot be solved analytically. It is necessary to use numerical methods, which was done using MATLAB software.

### 2.2 Structure of the Pole Placement controller

A controller based on the assignment of poles in a closed feedback control loop is designed to stabilize the closed loop while the characteristic polynomial should have previously determined poles [13]. This controller design comes from the general closed loop block diagram shown in Fig. 3, where:

\[ G_p(z) = \frac{Y(z)}{U(z)} = \frac{B(z^{-1})}{A(z^{-1})} \]  

(6)

is the discrete transfer function of the controlled plant with polynomials

\[ A(z^{-1}) = 1 + a_1 z^{-1} + a_2 z^{-2} \]

\[ B(z^{-1}) = b_1 z^{-1} + b_2 z^{-2} \]  

(7)

\[ G_R(z) = \frac{U(z)}{E(z)} = \frac{Q(z^{-1})}{P(z^{-1})} \]  

(8)

is the transfer function of a controller with polynomials

\[ P(z^{-1}) = (1 - z^{-1})(1 + \gamma z^{-1}) \]

\[ Q(z^{-1}) = q_0 + q_1 z^{-1} + q_2 z^{-2} \]  

(9)

From Eq. (8) it is possible to determine the controller equation in the form

\[ U(z) = \frac{Q(z^{-1})}{P(z^{-1})} E(z) \]  

(10)

and by inserting polynomials (9) into equation (10), the relation to calculate the controller output becomes
Further, the following relation can be obtained for the control transfer function of the closed loop shown in Fig. 3.

\[ u_k = q_0 e_k + q_1 e_{k-1} + q_2 e_{k-2} + (1 + \gamma) u_{k-1} + \gamma u_{k-2} \]

Figure 3. Block diagram of control loop for a PIDPP controller

\[ G_w(z) = \frac{Y(z)}{W(z)} = \frac{B(z^{-1})Q(z^{-1})}{A(z^{-1})P(z^{-1}) + B(z^{-1})Q(z^{-1})} \]  \hspace{2cm} (11)

where the characteristic polynomial is to be found in the denominator of (11). By choosing the characteristic polynomial

\[ D(z^{-1}) = 1 + \sum_{i=1}^{n_d} d_i z^{-i}, \quad n_d \leq 4 \]  \hspace{2cm} (12)

in the polynomial equation

\[ A(z^{-1})P(z^{-1}) + B(z^{-1})Q(z^{-1}) = D(z^{-1}) \]  \hspace{2cm} (13)

the desired pole placement for the transfer function is fixed (11). This is achieved by selecting the correct parameters for controller polynomials (10) which are the solution to polynomial equation (13). Detailed description of this controller is given in [13].

The positions of the poles vary according to the position of the operating point due to the system nonlinearity. It has a strong influence on the stability of the system. Therefore it is necessary to use the estimated values generated from the online system identification. The poles and zeros location of our system are further discussed in [14].

3 Results Section

The goal of the proposed method in this paper is to process the largest amount of filter cake in the shortest possible time. In contrast to the previously used approach, this new control design is newly extended by the controller to control the temperature of cooling water. Temperature of the coolant was set constant in the previous method, now it is controlled in the range from 283 to 323 K.

Processing of the filter cake is faster at higher temperature; therefore the setpoint is set to 370 K (Fig. 4).

Fig. 4. In-reactor temperature, coolant temperature and reactor filling up profiles

On the other hand, temperature must not exceed this value for safety reasons. It can be seen that the setpoint is changed from 370 K to 323.15 K in time 14,403 s. At this point all filter cake is processed and feeding is stopped. The entire process is completed at the time when the temperature falls to 323.15 K which was the initial temperature inside the reactor.

Fig. 5 shows the sudden change of manipulated variables especially at the beginning of the process. These changes are seen in the following graph (Fig. 6). Initially, appropriate heating of the reaction mixture is necessary due to the start of a chemical reaction. After that the reaction mixture must be cooled because of highly exothermic nature of this type reaction. Comparison of temperature profiles current and previously used method is shown in Fig. 7. It can be seen that adding a second controller, the duration of processing the same amount of filter
cake is significantly reduced. The total processing time of one batch is 25 460 s in case of one controller and 22 373 s in case of two controllers. The difference is 3 087 s.

Figure 6. Manipulated variables – detailed view

4 Conclusion
The semi-batch reactor control is a complex and difficult problem. Problems arise especially from its nonlinearity connected with a wide control range. Controllers must be able to deal with different stages (heating up, steady state). In this study, the PIDPP controllers for the temperature control of cooling water and for the feeding flow rate of a filter cake in a semi-batch reactor was demonstrated by simulation means. The implemented control strategy was also compared with another strategy applied on the same process in the previous works. Based on presented results it can be concluded that proposed method using two manipulated variables significantly reduces the time required to process one batch which can be seen in Figure 7.

There are still some other methods, which could possibly improve this process. In the future work, some other approaches will be applied to the batch process to find out other possible ways.

This work has been supported by the Tomas Bata University under grant IGA/FAI/2012/058. These supports are gratefully acknowledged.

References:
6th WSEAS International Conference on
Applied Informatics and Communications,
Elounda, Greece, 345-348.

Simulation Analysis of a Semi-Batch Reactor“
International Review of Automatic Control,
vol.2, no. 5, ISSN 1974-6059, 584-591.

equation parameters for control purposes, 13th
WSEAS International Conference on
Automatic Control, Modelling & Simulation
(ACMOS '11), WSEAS Press, 337-340.

preparation of regenerate for tanning. PhD.

2005, Digital Self-tuning Controllers, Springer,

reactor for control purposes. 22nd European
Conference on Modelling and Simulation,
Proceedings. European Council Modelling &