BATCH REACTOR ANALYSIS IN VIEW OF CONTROL THEORY

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ABSTRACT
In this paper, a control system design oriented analysis of a batch reactor used for tanning waste recovery is presented. The analysis is performed with the help of modelling and simulation means and provides useful information for optimal control design of the process.
Keywords: exothermic semi-batch reactor, modelling, analysis, simulation

1. INTRODUCTION

This paper deals with an analysis of a chemical reactor for chromium sludge (chromium filter cake) from tannery waste recovery. The reactor is used for the enzymatic hydrolysis product processing and the analysis is performed from the control theory point of view by simulation means mainly to obtain useful information for subsequent optimal control design.

2. A SEMI-BATCH REACTOR

The chromium sludge is processed in a chemical reactor by an exothermic chemical reaction with chrome sulphate acid [1]. During this reaction a considerable quantity of heat is developing so that control of the reaction is necessary. In order to investigate main properties of the real process, a mathematical model of the chemical reactor was derived based on Fig.1 [2,3].
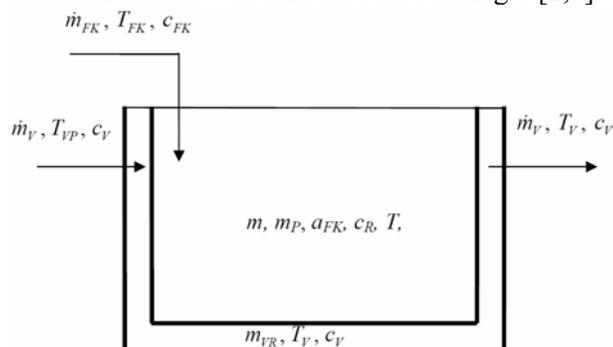
Figure 1. Chemical Reactor Scheme

2.1. Mathematical model

Under usual simplifications, based on the mass and heat balance, the following 4 nonlinear ordinary differential equations can be derived [2,3]:

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

$$\dot{m}_{FK} = k\, m(t)\, a_{FK}(t) + \frac{d}{dt}[m(t)\, a_{FK}(t)] \tag{1}$$

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

$$\dot{m}_V c_V T_{VP} + K\, S[T(t) - T_V(t)] = \dot{m}_V c_V T_V(t) + m_{VR} c_V \frac{d}{dt} T_V'(t)$$

The first equation expresses the total mass balance of the chemical solution in the reactor. The symbol $\dot{m}_{FK}$ [kg.s^{-1}] expresses the mass flow of the entering chromium sludge and $m'(t)$ [kg.s^{-1}] describes the accumulation of the in-reactor content.

The second equation represents the chromium sludge mass balance. The input is $\dot{m}_{FK}$ [kg.s^{-1}] again, the accumulation is given by the last term $[m(t)\, a_{FK}(t)]'$ [kg.s^{-1}], where $a_{FK}(t)$ [−] denotes the mass concentration of the chromium sludge in the reactor and $m(t)$ [kg] describes weight of the reaction components in the system. The expression $k\, m(t) a_{FK}(t)$ [kg.s^{-1}] defines the chromium sludge extinction by the chemical reaction. Here, k [s^{-1}] is the reaction rate constant expressed by the Arrhenius equation (2) where A [s^{-1}], E [J.mol^{-1}] and R [J.mol^{-1}.K^{-1}] are pre-exponential factor, activation energy and gas constant respectively.

$$k = A\, e^{-\frac{E}{RT(t)}} \tag{2}$$

The third equation describes the enthalpy balance. The input heat entering the reactor in the form of the chromium sludge is expressed by the term $\dot{m}_{FK} c_{FK} T_{FK}$, the heat arising from the chemical reaction is given by the expression $\Delta H_r k\, m(t) a_{FK}(t)$ and the heat transmission through the reactor wall is expressed by the formula $K\, S[T(t) - T_v(t)]$. The individual symbols used above mean: c_{FK} [J.kg^{-1}.K^{-1}] – chromium sludge specific heat capacity, c_R [J.kg^{-1}.K^{-1}] – specific heat capacity of the reactor content, 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 a coolant in the reactor double wall.

The last equation describes coolant heat balance. The input heat is given by $\dot{m}_v c_v T_{vp}$, the heat entering the coolant by the reactor wall is expressed by $K\, S[T(t) - T_v(t)]$, the heat going out with the coolant is described as $\dot{m}_v c_v T_v(t)$ and the heat accumulated in the double wall describes the last term $m_{vR} c_v T_V'(t)$. The symbols mean: $\dot{m}_v$ [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.

3. CONTROL THEORY POINT OF VIEW

From the systems theory point of view the reactor has four input signals $\dot{m}_{FK}(t)$, $\dot{m}_v(t)$, $T_{FK}(t)$ and $T_{vp}(t)$, four state variables $m(t)$, $a_{FK}(t)$, $T(t)$, $T_v(t)$ and one output signal to be controlled given by the temperature inside the reactor $T(t)$. Hence, it can be generally seen as a Multi Input – Multi

Output (MIMO) system of 4th order. In addition it possesses strongly nonlinear behaviour. Practically, the only manipulated variables are input flow rates of the chromium sludge $\dot{m}_{FK}(t)$ and of the coolant $\dot{m}_v(t)$. Therefore, input temperatures of the filter cake $T_{FK}(t)$ and of the coolant $T_{vp}(t)$ can be alternatively seen as disturbances. For further analysis, the reactor model described by the system of differential equations (1) is transformed into a linear time-variant (LTV) system.

3.1. Linear model
Having generally a nonlinear model defined by a system of formulas
$$x'(t) = f\left[t, x(t), u(t)\right],\tag{3}$$
where $x(t)$ defines a vector of state-variables $\left[x_1(t) \quad x_2(t) \quad \cdots \quad x_n(t)\right]$, $u(t)$ vector of input variables $\left[u_1(t) \quad u_2(t) \quad \cdots \quad u_m(t)\right]$ and f is a nonlinear vector function $\left[f_1 \quad f_2 \quad \cdots \quad f_n\right]$, then the linear model in a given operating (steady-state) point $\left(u^s, y^s\right)$ can be generally obtained using formulae with constant matrices A, B. As the reactor embodies astatic behaviour, it is not possible to compute the matrices in a chosen (steady-state) operating point. However, the linearization can be performed generally, resulting in a time-variant system:
$$x'(t) = A(t)x(t) + B(t)u(t)\tag{4}$$
where the matrices $A(t)$, $B(t)$ are no longer constant but time-dependent. Using the formulas above, the originally nonlinear model of the reactor has been transformed into a linear time-variant model. Generally, output from a linear system with matrices C, D is defined as:
$$y(t) = Cx(t) + Du(t)\tag{5}$$

3.2. Transfer function
As the reactor analyzed in this contribution is astatic, the linearized model is time-dependent. Then the transfer function (t.f.) is also time-dependent:
$$\tilde{G}(s,t) = C\left(sI_n - A(t)\right)^{-1}B(t).\tag{6}$$
where s is the complex Laplace variable and I_n is the n-by-n identity matrix.
Since the system generally has one output $T(t)$ and 4 inputs $\dot{m}_{FK}(t)$, $\dot{m}_v(t)$, $T_{FK}(t)$, $T_{vp}(t)$, the resultant t.f. is a vector of the 1-by-4 size:
$$\tilde{G} = \left[G_{T/\dot{m}_{FK}} \quad G_{T/\dot{m}_v} \quad G_{T/T_{FK}} \quad G_{T/T_{vp}}\right].\tag{7}$$
The first term $G_{T/\dot{m}_{FK}}$ describes the relation between the temperature inside the reactor $T(t)$ and the input flow rate of the chromium sludge $\dot{m}_{FK}(t)$. The other terms describes the relations between the temperature and the variables $\dot{m}_v(t)$, $T_{FK}(t)$, $T_{vp}(t)$ respectively. As stated earlier, the only practically manipulated variables are $\dot{m}_{FK}(t)$ and $\dot{m}_v(t)$. The transfer function for $\dot{m}_{FK}(t)$ has this general form (using (5) and (6)):
$$G_{T/\dot{m}_{FK}}(s,t) = \frac{B_3(t)s^3 + B_2(t)s^2 + B_1(t)s + B_0(t)}{s\left(s^3 + A_2(t)s^2 + A_1(t)s + A_0(t)\right)}\tag{8}$$

From the equation presented above, it can be seen that the relation between $T(t)$ and $\dot{m}_{FK}(t)$ is generally integrative. At present, the only practically manipulated variable is $\dot{m}_{FK}(t)$, therefore, the further investigation is focused on the analysis of the transfer function $G_{T/\dot{m}_{FK}}$.

3.3. Transfer function coefficients range
In order to determine the range of $G_{T/\dot{m}_{FK}}$ coefficients, a series of simulation experiments were performed in the MATLAB/Simulink environment. Some of the coefficients are very small and consequently they could be possibly neglected for the control system design.

3.4. Poles and zeros

Given the range of coefficients, it is possible to compute also the range of poles and zeros of $G_{T/\dot{m}_{FK}}$.

Results are summarized in Table 1.

Zeros at (or very close to) the origin indicate derivative behaviour whereas poles at the same position signalize integrative properties. The table shows that one pole (p_1) is directly at the origin resulting in integrative behaviour of the temperature $T(t)$ with respect to $\dot{m}_{FK}(t)$.

Table 1. Range of Poles and Zeros

z_i / p_i	Real min.	Real max.	Imag. min.	Imag. max.
z_1	0.0185	0.1601	0	0
z_2	-0.0062	-0.0062	0	0
z_3	-1.973×10^{-5}	0.0016	0	0
p_1	0	0	0	0
p_2	-0.0226	-0.0059	0	5.590×10^{-4}
p_3	-0.0067	0.0021	-5.590×10^{-4}	9.108×10^{-4}
p_4	-0.0018	8.464×10^{-4}	-9.108×10^{-4}	0

If the poles are located in the left part of the complex plane (their real parts are negative), the system is stable. From this point of view the table shows that generally the system embodies also instability. In addition, when the poles are complex (they also have imaginary parts), it indicates oscillatory behaviour. As revealed by the table, in some conditions the system may embody oscillatory behaviour, however absolute values of complex parts of the poles are relatively small which shows that this effect is not so significant. From the results, it can be also deduced that the system possesses non-minimum phase (NMP) behaviour – some of the zeros may become positive (unstable). Generally, NMP-systems are more difficult to control.

4. CONCLUSION

This contribution was focused on the analysis of a reactor used for the tanning waste recovery. The analysis was made by both theoretical and simulation means in order to provide useful information for optimal controller design. Havig the approximate uncertainty intervals of the coefficients, it suggests using the robust control approach [4]. As parameters of the linearized model change, an alternative idea could also be the usage of adaptive control strategies [5]. Another possible approach which proved to be successful is the predictive control [6].

5. ACKNOWLEDGEMENT

6. REFERENCES

[1] Kolomaznik, K., Mladek, M., Langmaier, F., Taylor, M., Diefendorf, E.J., Marmer, W.N., Tribula, E.: CR Patent 280655, Czech Republic, 1996.
[2] Macků, L.: Control design for the preparation of regenerate for tanning. PhD. Thesis, UTB in Zlin, Czech Republic, 2004 (in Czech).
[3] Macků, L.: "Modeling of tanning salts regeneration process." In Proceedings of the 15th Int. Conf. Process Control 2005 (High Tatras, Slovakia, Jun.7-10). Bratislava: Slovak University of Technology, 127/1-127/4. 2005.
[4] Morari, M., Zafirou, E.: Robust Process Control. Prentice Hall, Englewood Cliffs, New Jersey. 1989.
[5] Åström, K.J., Wittenmark, B.: Adaptive Control. Addison-Wesley, Reading, MA. 1989.
[6] Sámek, D., Macků, L.: "Simulation of model predictive control of semi-batch reactor." In Proc. Int. Symp. on Systems Theory SINTES 13 (Craiova, Romania, Oct.18-20). Craiova: University of Craiova, 180-185. 2007.