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CHEMICAL BATCH REACTOR MODELLING AND CONTROL

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ABSTRACT
The paper presents a chemical batch reactor control mechanism design. A program for a computer simulation using a mathematical model of the real reactor was created. An experimental based data were filled to the program to trace the real process state variables dependencies. Different process control approaches were simulated and the results were discussed. The components dosage influence and the risks related to the process were also discussed.
Keywords: chromium waste, process modelling, batch reactor, temperature control

1. INTRODUCTION
The alternative waste free method of dealing with the chromium waste is an enzymatic hydrolysis [1,2]. This technique separates the chrome from the protein in the form of a chromium filter cake (chromium sludge). The chromium sludge can be processed in a chemical reactor (Fig. 1.) by an exothermic chemical reaction with chrome sulphate acid (1). The process output chemical is reusable as a tanning salt again. During the exothermic reaction a considerable quantity of heat is developing so the reaction control is necessary. The reactor temperature has to stay under a critical temperature; otherwise the reactor could be destroyed. On the other side we need to use the maximum reactor capacity to process the maximum waste amount in the shortest possible time (request on higher temperature during processing).

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

2. THE SYSTEM MODEL
The chemical reactor mathematical model was derived to simulate the real process [3]. In Fig.2., we can see a chemical batch reactor scheme. The initial reactor filling is the chemical solution without the chromium sludge (filter cake) and its weight is symbolized by m_P[kg]. The chromium sludge dosage $\dot{m}_{FK}\ [kg.s^{-1}]$ is used to the developing heat control. The process balance equations are shown in (2). 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 entering chromium sludge, $m'[t]$ the accumulation of the in-reactor content.

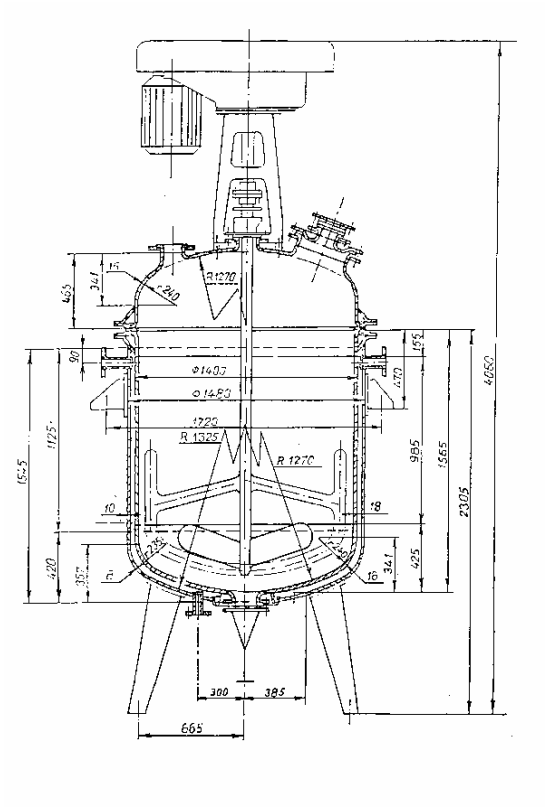

Figure 1. Chemical reactor.

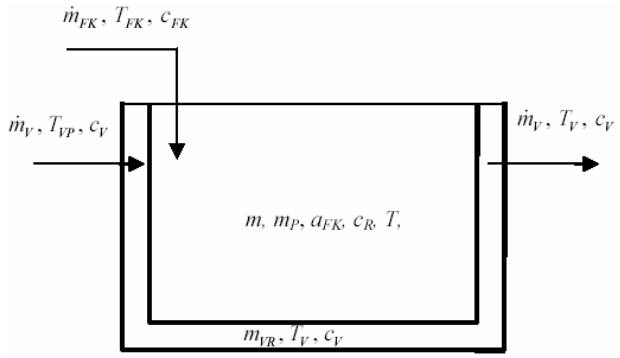

Figure 2. Scheme of chemical reactor.

$$\dot{m}_{FK} = m'[t]$$
$$\dot{m}_{FK} = m[t]\, a'_{FK}[t] + k\, m[t] a_{FK}[t]$$
$$\dot{m}_{FK} c_{FK} T_{FK} + \Delta H_r k\, m[t] a_{FK}[t] = K\, S\,(T[t] - T_V[t]) + m[t] c_R\, T'[t]$$
$$\dot{m}_V c_V T_{VP} + K\, S\,(T[t] - T_V[t]) = \dot{m}_V c_V T_V[t] + m_{VR} c_V\, T'_V[t] \qquad (2)$$

The second equation expresses the chromium sludge mass balance. The input is $\dot{m}_{FK}$ *[kg.s^{-1}]* again, the accumulation is $m[t]\, a'_{FK}[t]$ and the express $k\, m[t] a_{FK}[t]$ means the chromium sludge extinction caused by the chemical reaction. Symbol *k[s^{-1}]* means reaction rate constant expressed by the Arrhenius equation (3).

$$k = A e^{-\frac{E}{RT[t]}} \qquad (3)$$

$a_{FK}[t]$ means mass concentration of chromium sludge in the chemical reactor, $m[t]$*[kg]* 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 $\Delta H_r k\, m[t] a_{FK}[t]$ and the reactor wall heat transmission is $K\, S\,(T[t] - T_V[t])$. The individual symbols mean: c_{FK}*[J.kg.K^{-1}]* – chromium sludge specific thermal capacity, T_{FK}*[K]* – chromium sludge temperature, *ΔHr[J.kg^{-1}]* – heat of reaction, *K[kg.s^{-3}.K^{-1}]* - overall heat transfer 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 a coolant balance. The coolant input heat is expressed by $\dot{m}_V c_V T_{VP}$, the heat entering to the coolant from the reactor by the reactor wall is $K\, S\,(T[t] - T_V[t])$, the heat leaving with the coolant is $\dot{m}_V c_V T_V[t]$ and the heat accumulated in the double wall coolant expresses

$m_{VR} c_V T_V'[t]$. The symbols mean: $\dot{m}_V$ *[kg.s^{-1}]* – coolant mass flow, c_V*[J.kg.K^{-1}]* - coolant specific thermal capacity, T_{VP}*[K]* – input coolant temperature, m_{VR}*[kg]* – weight of the coolant mass in the reactor double wall. The symbol [*t*] after some symbols indicates that the symbols are function of time.

After rearranging (2) and replacing symbol *k* by (3) we obtain set of nonlinear differential equations (4), where all derivations of system state variables are on the left side. Variables $\dot{m}_{FK}, \dot{m}_V, T_{FK}, T_{VP}$ are actuating signals. Nevertheless, it is useful to choose only $\dot{m}_{FK}$, eventually $\dot{m}_V$ as actuating signals for the practical use. The temperature T_{FK} or T_{VP} change is inconvenient because of economical reasons (great energy demands).

$$
\begin{aligned}
m'[t] &= \dot{m}_{FK} \\
a'_{FK}[t] &= \frac{\dot{m}_{FK}}{m[t]} - A e^{-\frac{E}{RT[t]}} a_{FK}[t] \\
T'[t] &= \frac{\dot{m}_{FK} c_{FK} T_{FK}}{m[t] c_R} + \frac{A e^{-\frac{E}{RT[t]}} \Delta H_r \, a_{FK}[t]}{c_R} - \frac{K S T[t]}{m[t] c_R} + \frac{K S T_V[t]}{m[t] c_R} \\
T_V'[t] &= \frac{\dot{m}_V T_{VP}}{m_{VR}} + \frac{K S T[t]}{m_{VR} c_V} - \frac{K S T_V[t]}{m_{VR} c_V} - \frac{\dot{m}_V T_V[t]}{m_{VR}}
\end{aligned}
\qquad (4)
$$

Equations (4) were substituted by numeric values and simulated in the "Mathematica 4.1" software.

3. SIMULATIONS

To the theoretical reaction heat authentication and to the reaction kinetic determination calorimetric experiments were done. The experimental heats of reaction varied between 1624,44–1961,29kJ.mol^{-1}, the average value was 1747, 43kJ.mol^{-1}. The velocity constant on the temperature dependence expressed by Arrhenius equation was found as:

$$k = A e^{-\frac{E}{RT}} = 219{,}588\, e^{-\frac{3604{,}4634}{T}} \qquad (5)$$

Simulations with these constants filled in the system model (4) were done in the "Mathematica" software: *A = 219,588 s^{-1}*, *E = 29967,5087 J.mol^{-1}*, *R = 8,314 J.mol^{-1}.K^{-1}*, c_{FK} *= 4400 J.kg.K^{-1}*, c_V *= 4118 J.kg.K^{-1}*, c_R *= 4500 J.kg.K^{-1}*, m_{VR} *= 220kg*, *ΔHr = 1392350 J.kg^{-1}*, *K = 200 kg.s^{-3}.K^{-1}*, *S = 7,36 m^2*, $\dot{m}_V$ *= 1 kg.s^{-1}*, T_{FK} *= 293,15K*, T_{VP} *= 288,15K*. The $\dot{m}_{FK}$ dosage varied from *0* to *3kg.s^{-1}*. Initial conditions: the initial weight corresponded to the weight of initial reactor filling and was $m[0] = m_P$ *= 1810 kg*, the initial chromium sludge mass concentration in the chemical reactor was $a_{FK}[0] = a_{FK0}$ *= 0*, initial reactor filling temperature $T[0] = T_0$ *= 323,15K* and initial coolant temperature $T_V[0] = T_{V0}$ *= 293,15K*. The desired in-reactor temperature value was set as *370K* (the safe in-reactor temperature was determined as *373,15K*).

Because of the velocity constant influence, the developing heat doesn't follow the actuating signal (the chromium sludge dosing) but it is delayed. The in-reactor chromium sludge concentration accumulates quickly but the in-reactor temperature rises very slowly until the chemical reaction starts up. This reaction feature can caused uncontrollable temperature developing and reactor damage as a result. This phenomenon has to be considered with care during the process control design.

Different methods were simulated to find out the suitable control method. The two-step control, two-step control with the transient overshoot penalty and predictive control methods were simulated. The best results were achieved by predictive control as you can see in Fig. 3. and Fig. 4. The two-step control was not suitable because the temperature got over the safe value, but the two-step control with the penalty showed very good results as well (Fig. 5., Fig. 6.).

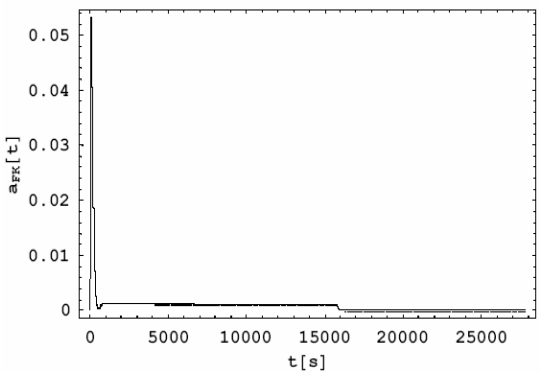

Figure 3. The in-reactor temperature development – predictive control

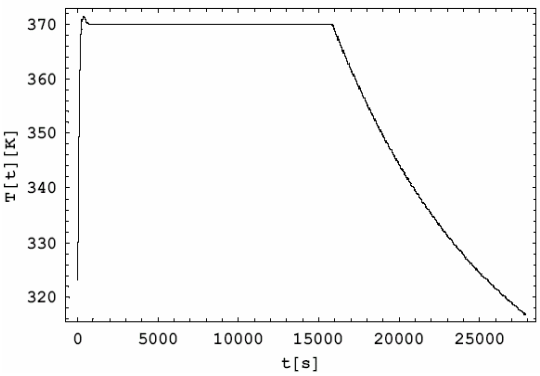

Figure 4. The in-reactor chromium sludge concentration development – predictive control

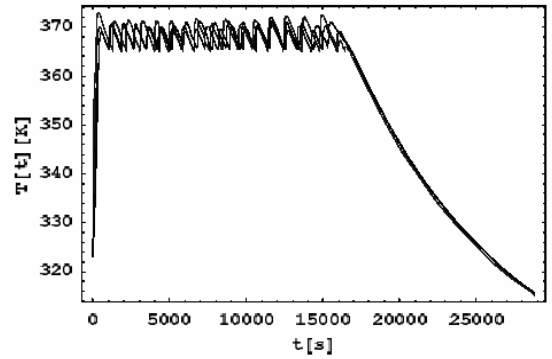

Figure 5. The in-reactor temperature development –two step control with the penalty

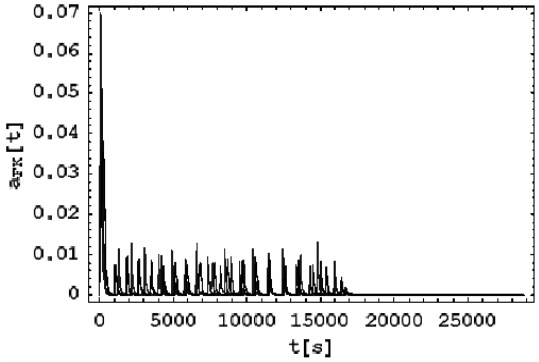

Figure 6. The in-reactor chromium sludge concentration development – two step control with the penalty

4. CONCLUSIONS

On the basis of the experiments and simulations was found out that industrial application of the chemical reactor using two-step control with the penalty is suitable enough and the costs of such an application should be less expensive than the predictive control application costs [4]. Some more details could be found out in a next research.

5. ACKNOWLEDGMENTS

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