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DIFFERENT APPROACHES TO CHEMICAL EXOTHERMIC BATCH REACTOR CONTROL

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ABSTRACT
The paper presents some different methods for a chemical exothermic batch reactor control. A mathematical model including reaction kinetics was used to simulate a real process. The process chemical 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 generally difficult by common methods.
Keywords: Predictive control, chemical batch reactor, process modelling, temperature control

1. INTRODUCTION
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 [1].
The interest in the control of batch reactors has increased in recent years because of the expansion of small-volume specialty chemicals. In the biotechnology area, batch reactors are used on both small- and largescale fermenters because of the inherent superiority of batch fermentation over continuous fermentation in most systems. Many of these batch reactors are “semibatch” or “fedbatch” reactors in which an initial amount of material is placed in the reactor, the liquid is heated to the desired temperature, and then additional feed of fresh reactant is gradually added to the vessel. The result is a time-varying process with variable volume. If heating and/or cooling is achieved by heat transfer from the vessel liquid into a heating/cooling medium in a surrounding jacket, the time-varying volume means that the heat-transfer area is also changing with time. The optimum operation of many fed-batch reactors is an operating strategy that minimized the batch time. This corresponds to feeding the

fresh feed into the reactor as quickly as possible. The feed rate is often limited by heat transfer. If the reaction is exothermic, heat must be removed. The rate of heat transfer depends on three factors [2]: 1. The temperature difference between the reaction liquid and the jacket coolant. The latter depends on the coolant flow rate, the inlet coolant temperature, and the heat-transfer rate. 2. The overall heat-transfer coefficient, which depends on agitator mixing in the vessel and the flow rate of coolant in the jacket. 3. The heat-transfer area. If jacket cooling is used, the effective heat-transfer area in a fed-batch reactor varies during the course of the batch directly with the volume of liquid in the vessel.
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 [3]: (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 different control approaches. The model input data comes from an real process - the chromium waste recycling process [4]. The model equations are (1-4):

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

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

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

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

The individual symbols in equations (1-4) mean: 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=29967,5087 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.
The fed-batch reactor use jacket cooling, but the effective heat-transfer area (S=7,36 m^2) in the mathematical model was treated as constant, not time varying. The initial amount of material placed in the reactor takes about two-thirds of the in-reactor volume and the reactor is treated as ideally stirred, so we can do this simplification.

3. CONTROL METHODS

Four different control methods vere simulated to control the fed-batch reactor – two step control, two step control with penalization, PID control, model predictive control using artificial neural network. The two step control without penalization was not satisfactory, so we skip that one. The task was to control the in-reactor temperature T by reaction component dosing F_I. The desired value of temperature T was 270K and the maximum value shouldn't exceed 273K. The actuating variable F_I was from the interval <0,3> kg.s^{-1}.

3.1. Two step control with penalization

The two step control with penalization provided these results: the upper-most in-reactor temperature T reached 372.93 K, the maximum chromium sludge concentration a was 0,0762 and the total batch time made 25727 seconds. The in-reactor temperature oscilated around the desired value in the subrange of 7 Kelvin degrees. The result process control diagrams are displayed in figure 1.

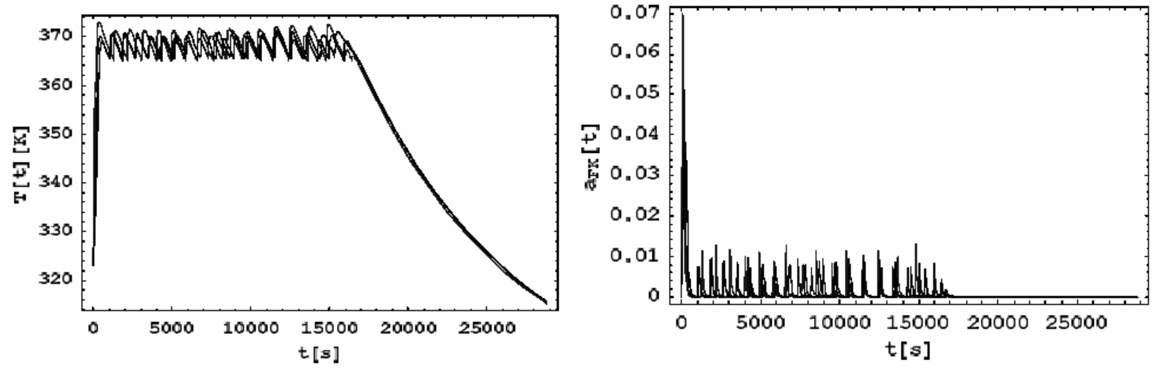

Figure 1. The in-reactor temperature and chromium sludge concentration development – two step control with penalization

3.2. PID control

The results of PID control were following: the upper-most in-reactor temperature T reached 370.22 K, the maximum chromium sludge concentration a was 0,0439 and the total batch time made 25491 seconds. The maximum end minimum actuating variable values were 1.546 kg.s^{-1} or 0 kg.s^{-1} respectively. The steady state actuating variable value made approximately 0,032 kg.s^{-1}. The PID control diagrams are displayed in figure 2.

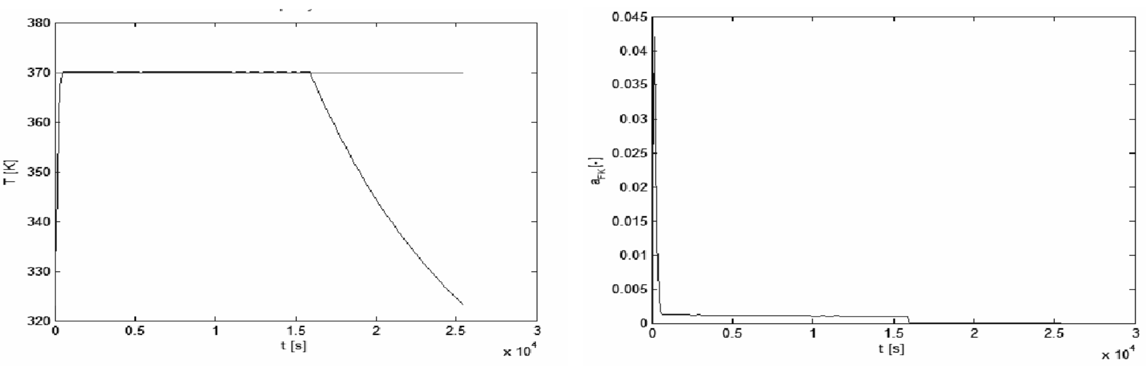

Figure 2. The in-reactor temperature and chromium sludge concentration development – PID control

3.3. Model predictive control

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 [5]. Generally we can say that MPC use artificial neural 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. Typical form of the performance criterion J is as follows:

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

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 ANN predictor response. The λ and ρ 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, the third part of the criterion was added where the γ parameter determines the contribution that the third sum has on the performance index. However, in order to avoid the permanent control error the γ parameter was during the control gradually decreased up to zero. In other words, the third sum in the beginning of the control has the maximum value, and after initial phase it equals to zero.

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

As can be seen from the figure 3, the MPC 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 end 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^{-1}.

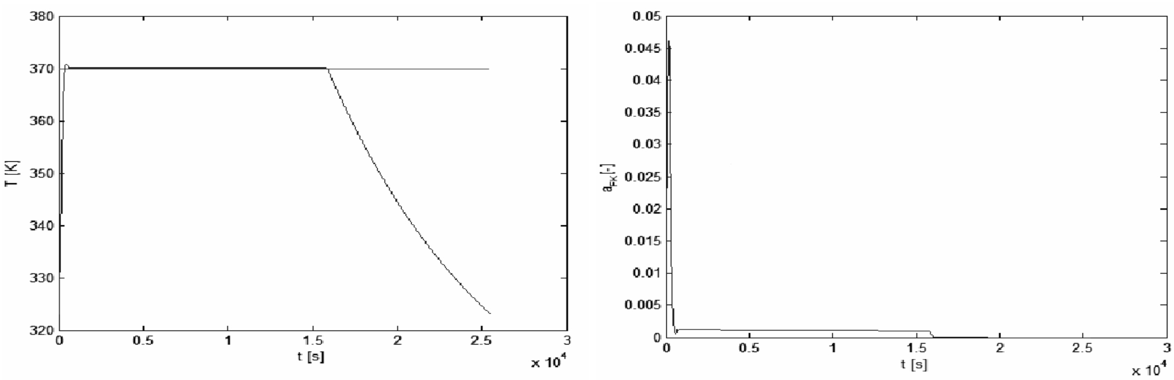

Figure 3. The in-reactor temperature and chromium sludge concentration development – MPC

4. CONCLUSION

It is difficult to distinguish which one of the shown control method was the best. The shortest process time provided the PID control method, but the difference with regard to MPC was only 8 seconds. The total process time took over 7 hours, so the difference 8 seconds can be neglected. The best control performance was obtained by MPC, but simulation of this method is quite hardware demanding today. The simulation using CPU 2500 MHz computer took almost 2 hours. The cheapest solution for an industrial application could be the two step control with penalization, but just in the case we don't need precise control performance.

5. ACKNOWLEDGEMENT

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