

## INFLUENCE OF REACTION KINETICS ON THE CHEMICAL BATCH PROCESS SAFETY

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### ABSTRACT

*In this paper, influence of reaction kinetics on an exothermic process running in a batch reactor is discussed. A first order exothermic chemical reaction is considered to be running in the reactor. A process model accounting this type of reaction was set up and used to trace the in reactor temperature development. The process model based on heat and mass balanced equations was simulated with the help of Mathematica software. The influence of reaction kinetics on the process safety and the temperature control performance are discussed.*

**Keywords:** reaction kinetics, modelling, chemical process, process control

### 1. INTRODUCTION

In fine chemical or pharmaceutical industry, the batch or fed-batch reactor functions as the heart of the process transformation. Due to the complexity of the reaction mixture and the difficulty to perform on-line composition measurements, control of batch reactors is essentially a problem of temperature control [1]. The amount of released heat can become very large as the reaction mixture is heated up, very quickly the reaction may become unstable and cause the temperature to run away if the heat generated exceeds the cooling capacity of the reactor. This runaway can seriously cause risk to plant personnel and equipment and can, even in the best case, result in loss of the batch. Therefore, careful control of the rate of change of the reactor temperature and minimization of the temperature overshoot is required. On the other hand, from the production point of view, the heat up should be done as quickly as possible in order to reduce the overall cycle time of the reaction process. Therefore, any control strategy must balance the needs of production with use of safety and quality. Influence of reaction kinetics on an exothermic process running a first order exothermic chemical reaction is considered in this paper. The process model accounting this type of reaction is described further.

### 2. PROCESS MODEL

The scheme of the batch reactor is depicted in Fig. 1. and the model is described by equations (1-4) [2].

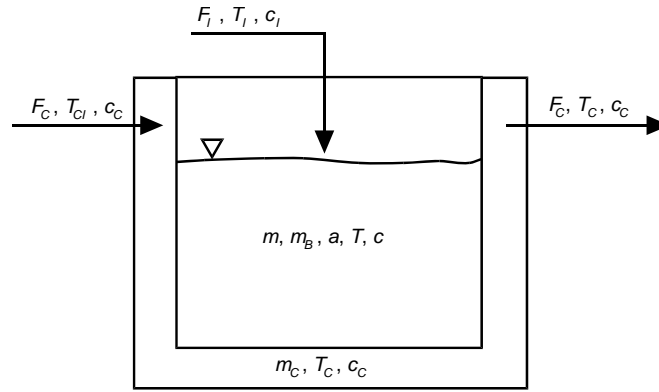


Figure 1. The batch reactor scheme

The task is to control the in-reactor temperature  $T$  by reaction component dosing  $F_I$ . The desired value of temperature  $T$  is 270K and the maximum value shouldn't exceed 273K. The actuating variable  $F_I$  has to be in the interval  $\langle 0,3 \rangle \text{ kg}\cdot\text{s}^{-1}$ . The other data used for the batch reactor modelling were counted for the chromium waste recycle process [3] or estimated.

$$\frac{dm(t)}{dt} = F_I \quad (1)$$

$$\frac{da(t)}{dt} = \frac{F_I}{m(t)} - A \cdot e^{-\frac{E}{R \cdot T(t)}} \cdot a(t) \quad (2)$$

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

$$\frac{dT_C(t)}{dt} = \frac{F_C \cdot T_{CI}}{m_C} + \frac{K \cdot S \cdot T(t)}{m_C \cdot c_C} - \frac{K \cdot S \cdot T_C(t)}{m_C \cdot c_C} - \frac{F_C \cdot T_C(t)}{m_C} \quad (4)$$

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,  $c=4500 \text{ J}\cdot\text{kg}\cdot\text{K}^{-1}$  is the specific heat capacity of the reactor content,  $T$  is the temperature of the reactor content.  $F_I, T_I=293,15 \text{ K}$  and  $c_I=4400 \text{ J}\cdot\text{kg}\cdot\text{K}^{-1}$  is the reaction component input mass flow rate, temperature and specific heat capacity.  $F_C=1 \text{ kg}\cdot\text{s}^{-1}$ ,  $T_{CI}=288,15 \text{ K}$ ,  $T_C, c_C=4118 \text{ J}\cdot\text{kg}\cdot\text{K}^{-1}$  and  $m_C=220 \text{ kg}$  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:  $A=219,588 \text{ s}^{-1}$ ,  $E=29967,5087 \text{ J}\cdot\text{mol}^{-1}$ ,  $R=8,314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ ,  $\Delta H_r=1392350 \text{ J}\cdot\text{kg}^{-1}$ ,  $K=200 \text{ kg}\cdot\text{s}^{-3}\cdot\text{K}^{-1}$ ,  $S=7,36 \text{ m}^2$ .

## 2.1. The velocity konstant

In equations (2) and (3) is included influence of temperature and reaction component mass concentration on the reaction rate. The temperature dependence is defined by Arrhenius equation (5), where  $k$  is the velocity constant:

$$k = A e^{-\frac{E}{RT[t]}} \quad (5)$$

The velocity constant causes an accumulation of the reaction component in the reactor without corresponding temperature rise. Then, the level of concentration which starts the reaction is reached and the reaction runs very fast. The temperature rises as well and causes the reaction runs even faster. Thus, if the amount of non-reacted reaction component in the reactor is too high, the temperature

became uncontrollable and we can't avoid its overshooting. An example of the overshoot caused by accumulation you can see in figure 2. In the left plot you can see a temperature overshoot over 373K, which was caused by the accumulation of the reaction component. The corresponding mass concentration is depicted in the right plot. The plots were obtained by a two step control simulation. The actuating signal switch-off was set on 370K, the switch-on was set on 365K. In the steady state (from approximately  $t = 2000s$ ) was the control performance satisfactory. So, it is necessary to take into account the mass concentration to prevent the temperature overshooting. With the knowledge of the above-mentioned model, we can find the safe value of the reaction component concentration during the start-up part of the process control (figure 3.) and so prevent the temperature overshooting.

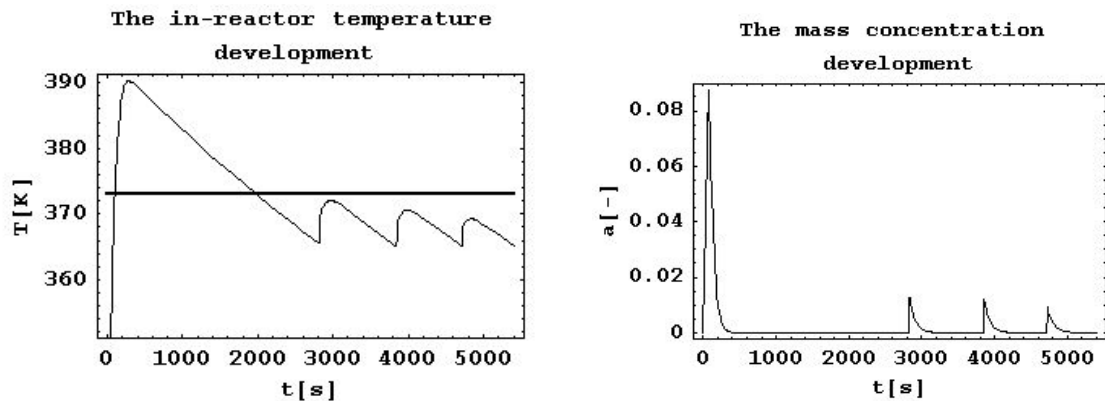


Figure 2. The in-reactor temperature development and the corresponding mass concentration development

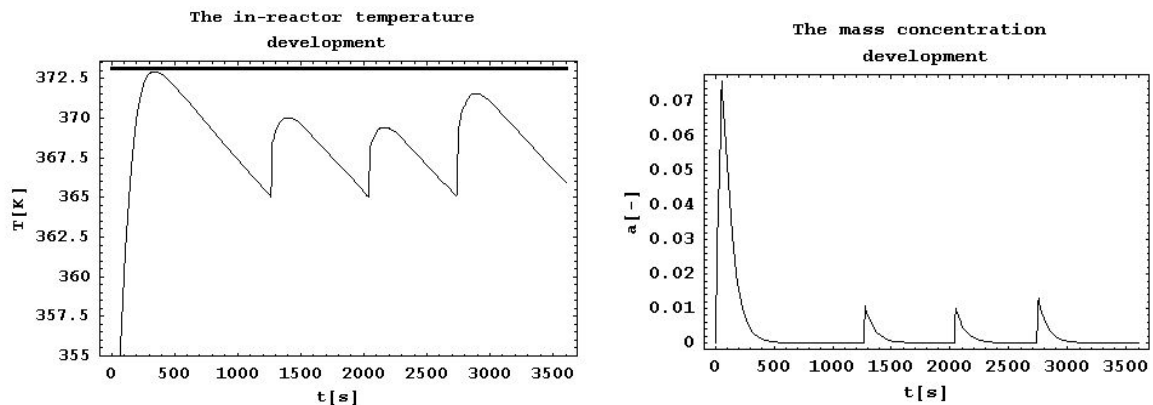


Figure 3. The in-reactor temperature development and the corresponding mass concentration development – penalized values

Plots show simulation of two-step control with the temperature and reaction component penalization. In case the reaction component mass concentration reach the set value and the temperature gets over penalized value at the same time the actuating variable  $F_I$  is switched off. The non-reacted chromium sludge is so prevented from cumulating in the chemical reactor. The insensitivity zone was chosen at interval  $(T_{PP} + 1 > T[t] \geq T_{PP})$ , to prevent the in-reactor temperature to oscillate around the penalty temperature. The penalty values were set on the basis of simulations experiences as follows:

$$\begin{array}{lll}
 F_I = 0,5: & T_{PP} = 362K, & a_{PP} = 0,02 \\
 F_I = 1: & T_{PP} = 357K, & a_{PP} = 0,02 \\
 F_I = 3: & T_{PP} = 353K, & a_{PP} = 0,02
 \end{array}$$

The process control diagrams are displayed on figures 4-5 and the summary of obtained values in the table 1.

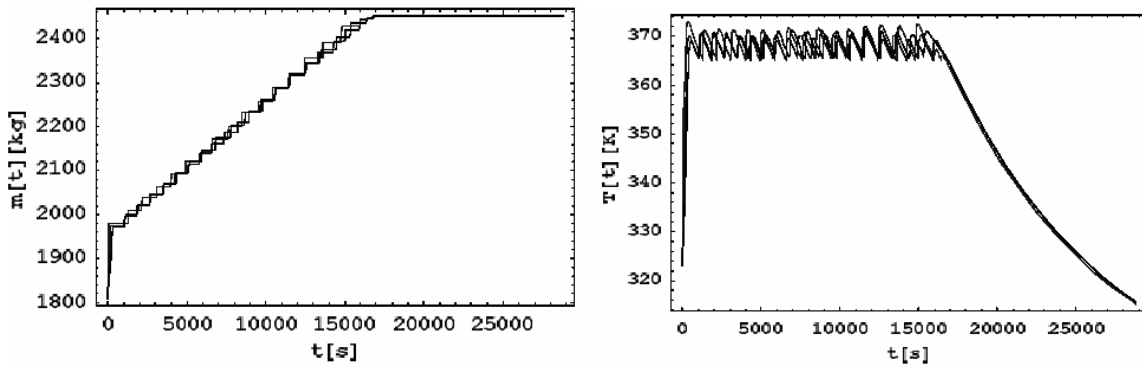


Figure 4. The in-reactor weight and temperature development

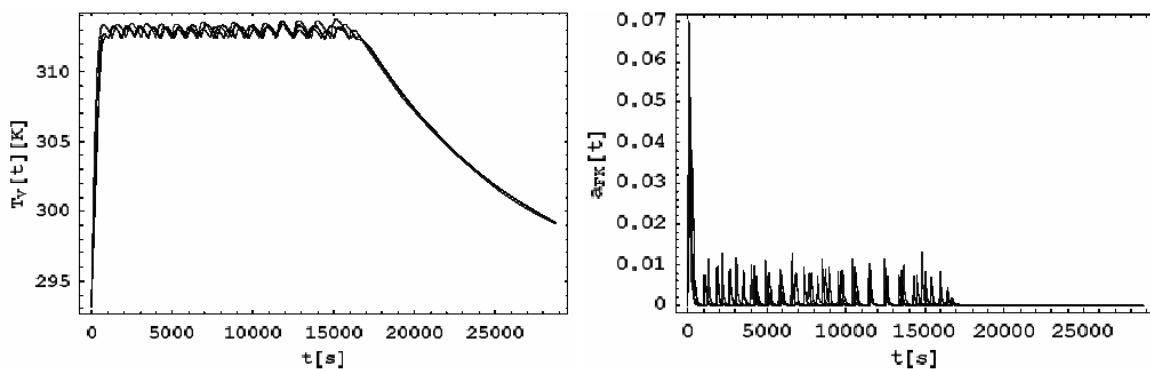


Figure 5. The coolant temperature and the in-reactor chromium sludge concentration development

$F_I$ [kg.s <sup>-1</sup> ]	$T_{max}$ [K]	$T_c$ [K]	$a_{max}$ [-]	$t_{total}$ [s]	$t_{total}$ [h,m,s]
0,5	371,13	313,41	0,0354	25889	7,11,29
1	372,01	313,61	0,0528	25886	7,11,29
3	372,93	313,72	0,0762	25727	7,8,47

Table 1. Values obtained during the penalized two-step control.

### 3. CONCLUSION

The performed simulations demonstrate the importance of the process modelling, and its impact on the process control performance and safety. With the right built-up model we can even with simple control approach obtain satisfactory results and predict the process behaviour. This can lead to overall process timesaving and better process efficiency.

### 4. ACKNOWLEDGEMENT

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### 5. REFERENCES

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