

# Experimental identification of Arrhenius equation parameters for control purposes

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*Abstract:* - In the process control area, there are a lot of systems with nonlinear behaviour. Specific case of such nonlinear system is an exothermic chemical reactor. The reactor nonlinearity can arise from different reasons. One of them is the changeable reaction speed, which depends on the reactants concentration and the in-reactor temperature. The second dependence is described by Arrhenius equation. Knowledge of the Arrhenius equation parameters is a key for correct mathematical model composition and also for safe and successful control. Some possibilities of the parameters determination are described in the literature. However, they are complicated and not very suitable for online identification of a real process. A new approach developed by the author is introduced in this article. The possibility of identification the reaction rate and its temperature dependence from a measured temperature profiles are shown. The identification method including all necessary derivation is described. Also the results of experimentally measured data identification are presented.

*Key-Words:* - rate constant, exothermic process, semi-batch reactor, identification, simulation, control

## 1 Introduction

The interest in the control of batch reactors has increased in recent years because of the expansion of small-volume specialty chemicals. Many of these batch reactors are “semibatch” or “fedbatch” reactors in which an initial amount of material is placed in the reactor, the content 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 [1]: 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 [2]: (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.

The in-reactor temperature control may be complicated by reaction kinetics. The heat released by chemical reactions is function of the reaction rate. The reaction rate depends on individual reactants concentrations and also on the system temperature. The temperature dependence is described by Arrhenius equation. Influence of this equation on the batch process control and possibility of its parameters determination are studied in this paper.

## 2 Semi-batch chemical reactor model

This study deals with influence of reaction kinetics on an exothermic process running a first order

reaction, so in this section a mathematical model of such system is described.

Let us consider single input – single output (SISO) system of chemical exothermic semi-batch reactor (figure 1). The reactor has a double wall for cooling medium and we consider that its content is ideally stirred.

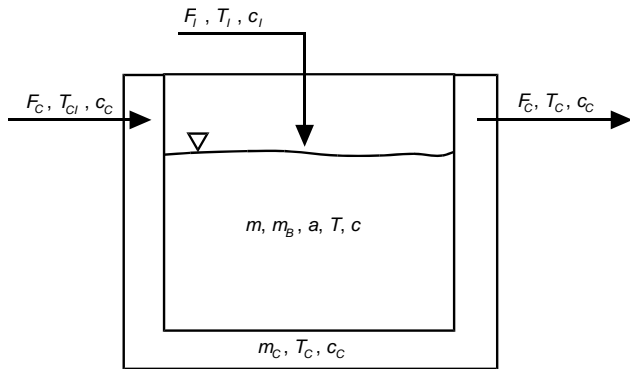


Fig. 1 Exothermic semi batch reactor scheme.

The scheme above shows a chemical semi-batch reactor with initial filling  $m_B$  [kg] given by the solution of chemicals. A reactant causing an exothermic chemical reaction to run is fed into the reactor to control the developing heat. The temperature has to stay under a certain critical level; otherwise the reactor could be destroyed. It is also desirable to utilize the whole capacity of the reactor to process the maximum amount of chemicals in the shortest possible time (higher temperature is desirable). Therefore an optimal control strategy has to find a trade-off between these opposite requirements – higher temperature for faster processing contra lower temperature for process safety.

After applying usual simplifications the mathematical model of this system can be written by equations (1)-(4).

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

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

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

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

$$\frac{K \cdot S \cdot T_C(t)}{m_C \cdot c_C} - \frac{F_C \cdot T_C(t)}{m_C} \quad (4)$$

The used model was set up for the chromium waste recycle process [3,4,5], so for simulations were taken the parameters of this process. Here  $m$  is the total weight of reaction components in the reactor,  $a$  is the mass concentration of the reaction component in the reactor,  $c = 4500 \text{ J.kg.K}^{-1}$  is the specific heat capacity of the reactor content;  $T$  is the temperature of the reactor content.  $F_I, T_I = 293.15 \text{ K}$  and  $c_I = 4400 \text{ J.kg.K}^{-1}$  is the reaction component input mass flow rate, temperature and specific heat capacity.  $F_C = 1 \text{ kg.s}^{-1}$ ,  $T_{CI} = 288.15 \text{ K}$ ,  $T_C, c_C = 4118 \text{ J.kg.K}^{-1}$  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, respective ely. Other constants:  $A = 219.588 \text{ s}^{-1}$ ,  $E = 29967.5087 \text{ J.mol}^{-1}$ ,  $R = 8.314 \text{ J.mol}^{-1}.\text{K}^{-1}$ ,  $\Delta H_r = 1392350 \text{ J.kg}^{-1}$ ,  $K = 200 \text{ kg.s}^{-3}.\text{K}^{-1}$ ,  $S = 7.36 \text{ m}^2$ .

The fed-batch reactor use jacket cooling, but the effective heat-transfer area ( $S = 7.36 \text{ m}^2$ ) 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.

## 2.1 The rate constant

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 rate constant:

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

The rate 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 temperature overshoot caused by accumulation can be seen in figure 2. Here 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 figure 3. 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. It was impossible prevent the temperature overshooting and simultaneously to trace the desired value 373K. 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.

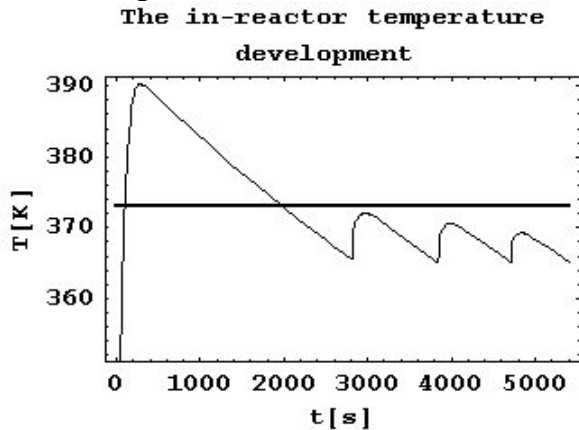


Fig. 2 The temperature overshoot caused by the reactant accumulation

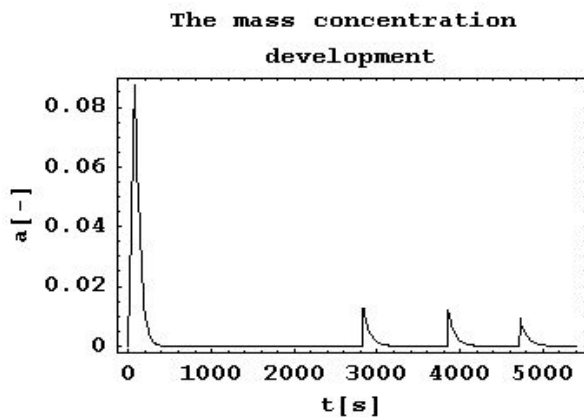


Fig. 3 The mass concentration development (control without penalization)

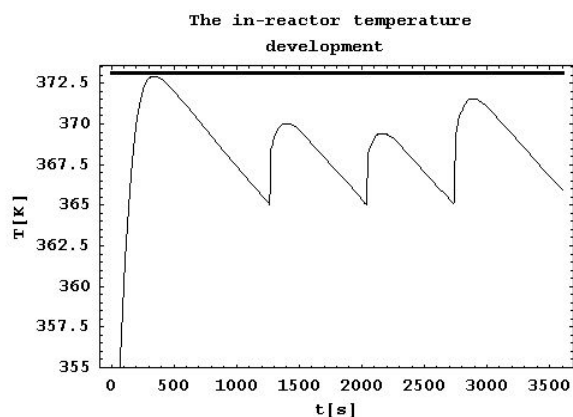


Fig. 4 The temperature development without overshoot – penalized values

With the knowledge of the previously mentioned model (that means also the knowledge of the rate constant) we can find the safe value of the reaction component concentration during the start-up part of the process control and so prevent the temperature overshooting as can be seen in figure 4. The corresponding mass concentration development is than showed in the figure 5.

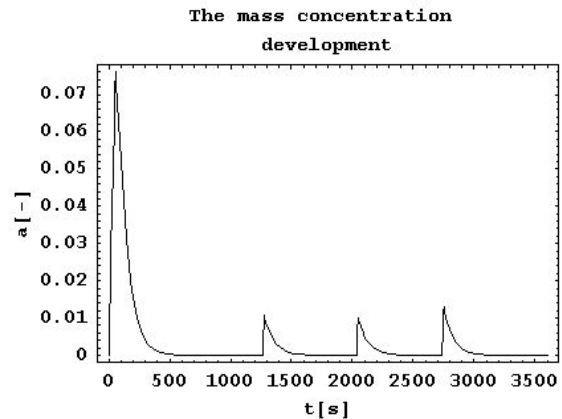


Fig. 5 The mass concentration development – penalized values

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 chemical reactant 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.

As can be seen from the above mentioned text, it is important to know the velocity constant parameters to be able satisfactory control like these processes. As far as we use the very same chemicals for processing, there is no generally problem. We can do the identification once and the parameters are always the same. But in case we plan processing wider range of chemicals, or the mixture properties are changeable in time, it is necessary to perform on-line velocity coefficient identification to process safely different mixture types.

### 3 Rate constant identification

In this chapter the procedure for the Arrhenius equation parameters identification is described.

The heat  $Q$  can be expressed by equation:

$$Q = C \Delta T_1 \quad (6)$$

where  $C$  is a system heat capacity (the heat needed for system warming up for 1 K) and  $\Delta T_1$  the system temperature increase caused by the generated heat.

As was mentioned before, we assume that the exothermic chemical reaction can be treated as a first order reaction from the reaction kinetic point of view. That means that the reaction velocity  $v$  is directly proportional only to one of the reactive components  $c$ , as can be seen in formula (7).

$$v = -dc/dt = kc \quad (7)$$

Here the symbols have the following meaning:  $v$  – reaction velocity,  $c$  – concentration of the reaction component,  $t$  – time,  $k$  – velocity constant. The velocity constant  $k$  can be generally determined by measurement of any property which is proportional to the concentration. Since we are interested in exothermic reaction, it seems to be possible to trace the amount of heat generated by the chemical reaction. This generated heat is adequate to number of reacted moles and so also to the concentration of the reaction component.

The equation (6) implies that the system temperature increase corresponds to the generated heat as can be seen from the equation below (8):

$$dT = \frac{dQ}{C} \quad (8)$$

We also know, that the increase of heat  $dQ$  released by the chemical reaction matches the product of reacted moles  $dn$  and heat of reaction  $\Delta H_r$ . It can be written:

$$dQ = \Delta H_r dn = dcV \Delta H_r \quad (9)$$

where the product of concentration changes and the volume of reaction mixture matches the number of moles. After dividing the equation (8) by time  $t$  and with the help of substituting equation (9) we obtain the relationship (10):

$$\frac{dT}{dt} = \frac{V \Delta H_r}{C} \frac{dc}{dt} \quad (10)$$

where the term  $dc/dt$  expresses the reaction rate, see relation (7). Putting (7) into (10) allows us to extrapolate the temperature derivative at zero time. We obtain the relationship:

$$v = -\frac{dT}{dt} \frac{C}{V \Delta H_r} \quad (11)$$

By comparing relations (11) with relation (7) we get the equation for rate constant:

$$k = \frac{dT}{dt} \frac{C}{V \Delta H_r c} = \frac{dT}{dt} \frac{C}{\Delta H_r n} \quad (12)$$

Individual symbols: derivation  $dT/dt$  means a tangent direction (see figure 6),  $C$  [J.K<sup>-1</sup>] – system thermal capacity,  $V$  [m<sup>3</sup>] – volume,  $c$  [mol.m<sup>-3</sup>] – molar concentration,  $n$  [mol] – the number of mole.

As can be seen from the formula (6) we need to know the in-reactor chemicals volume  $V$  and concentration of reactant causing the heat development  $c$  (or the number of mole  $n$  instead) to determine the rate constant. Further it is necessary to know also the heat of reaction  $\Delta H_r$ , system thermal capacity  $C$  and the temperature tangent direction  $dT/dt$ .

By substituting the experimentally observed data to the expression (12) we can calculate its value – the rate constant for the different initial reaction temperatures. The derivative  $dT/dt$  is actually tangent to the curve of  $T$  dependence as a function of  $t$ . The tangent value can be determined from the temperature-time graph, which is obtained by recording the temperature during a chemical reaction, see figure 6.

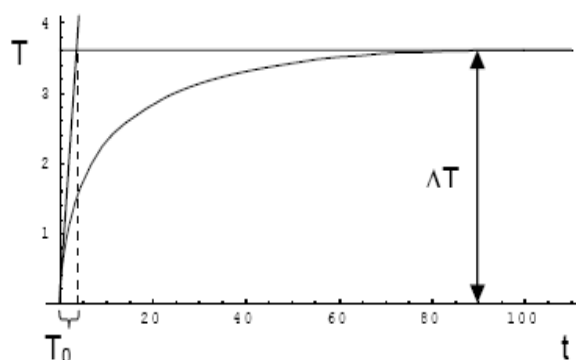


Fig. 6 An example of reaction temperature time dependence

It is advantageous to read the directive in the start of the reaction, because we know the initial concentrations of substances. Therefore the known initial concentration  $c_0$  can be put into relation (12) for the concentration  $c$ . The volume  $V$  of reaction

mixture is also known and the value of reaction heat  $\Delta H_r$  can be found experimentally.

To determine the rate constant temperature dependence we use the Arrhenius relationship in the shape of a logarithmic form (13):

$$\ln k = \ln A - \frac{E}{RT} \quad (13)$$

Plotting the dependence  $\ln k$  on  $1/T$  gives a linear dependence in the form  $y = a + b x$ . From this dependence we find values  $a$  and  $b$ . By comparing this dependence with the relation (13) we obtain for calculating pre-exponential factor  $A$  and activation energy  $E$  relationships:

$$A = e^a \quad (14)$$

$$E = -bR \quad (15)$$

These constants are used to compile the model equations of the chemical reactor.

## 4 Experiments evaluation

This section describes how to determine the coefficients of the Arrhenius equation from experimentally observed data.

### 4.1 Calculation of reaction heats

In this subsection the data obtained by

measurements in the experimental calorimeter are introduced. The data comes from 15 experiments and can be found in the table 1. For each experiment are always given an initial temperature  $T_I$  [°C] prior to chemical reaction, the final temperature  $T_F$  [°C] after the reaction and the difference  $\Delta T$  [K] of these temperatures. There are also stated the amounts of added chemicals  $n$  [mol] that cause the heat generation and the corresponding temperature rise. Also the measured calorimeter heat capacity  $C$  [J/K] is given.

Now we can calculate the reaction heats so that we substitute the temperature difference and specific heat capacity of calorimeter from the table 1 into the relationship (6). These counted reaction heats are also displayed in the table 1.

### 4.2 Rate constant and its temperature dependence estimating

For the calculation of rate constants we use relation (12). We need to know the value of tangent directions  $dT/dt$  first. They can be determined from the temperature curves at the beginning of experiments as was mentioned earlier. All the measured data are depicted in figures (7) to (21)

The tangent direction is evaluated in that way that a second-degree ( $y = fx^2 + gx + h$ ) polynomial interpolation of measured data is done first. After it, the polynomial is derived by zero time. So the tangent direction in the beginning of the reaction is obtained.

Table 1 Experimental data and the calculation of reaction heats

Number of experiment	Initial temperature $T_I$ [°C]	Final temperature $T_F$ [°C]	Temperature difference $\Delta T$ [K]	Heat capacity of calorimeter $C$ [J/K]	Number of moles of reactant $n$ [mol]	Heat of reaction $\Delta H_r$ [kJ/mol]
1	66.7	73.7	7.0	922.99	0.003557	<b>1805.39</b>
2	57.8	63.3	5.6	880.55	0.003557	<b>1382.67</b>
3	49.7	54.5	4.8	765.11	0.003557	<b>1027.23</b>
4	67.6	74.2	6.6	922.99	0.003571	<b>1716.47</b>
5	59.4	65.3	5.9	880.55	0.003592	<b>1454.27</b>
6	48.5	54.7	6.2	765.11	0.003521	<b>1342.79</b>
7	69.4	75.6	6.2	922.99	0.003535	<b>1629.57</b>
8	61.7	66.2	4.6	880.55	0.003585	<b>1124.56</b>
9	47.1	54.1	7.0	765.11	0.003542	<b>1503.97</b>
10	45.4	51.7	6.3	765.11	0.003514	<b>1364.07</b>
11	57.2	62.8	5.7	880.55	0.003585	<b>1398.97</b>
12	71.7	78.0	6.3	922.99	0.003564	<b>1624.44</b>
13	49.9	55.5	5.6	765.11	0.003599	<b>1182.70</b>
14	60.3	65.5	5.2	880.55	0.003542	<b>1283.15</b>
15	67.2	74.8	7.7	922.99	0.003606	<b>1961.29</b>

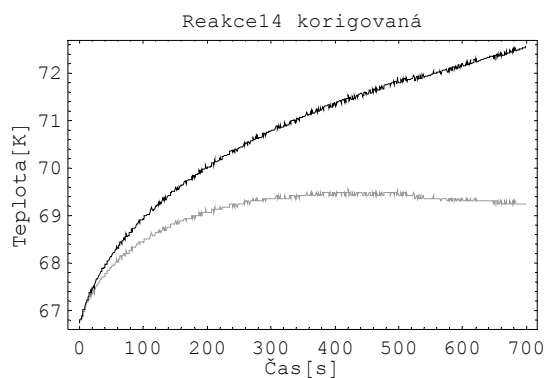


Fig. 7 Temperature course of the experiment number 1

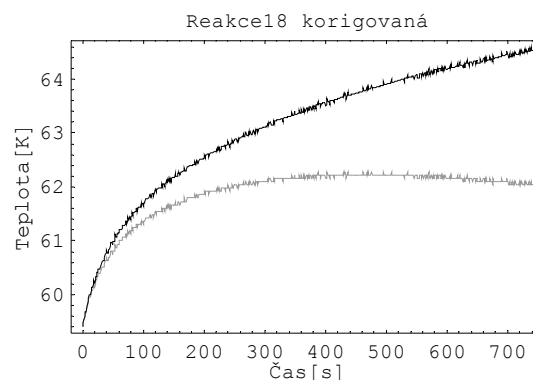


Fig. 11 Temperature course of the experiment number 5

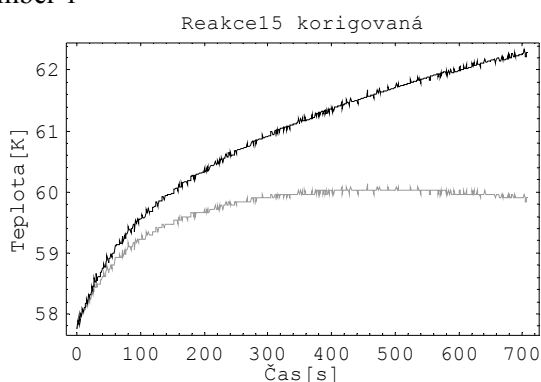


Fig. 8 Temperature course of the experiment number 2

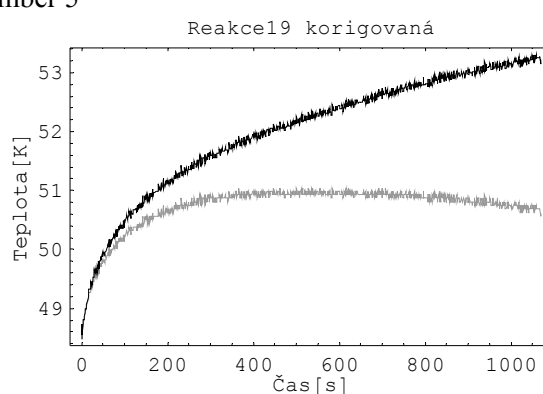


Fig. 12 Temperature course of the experiment number 6

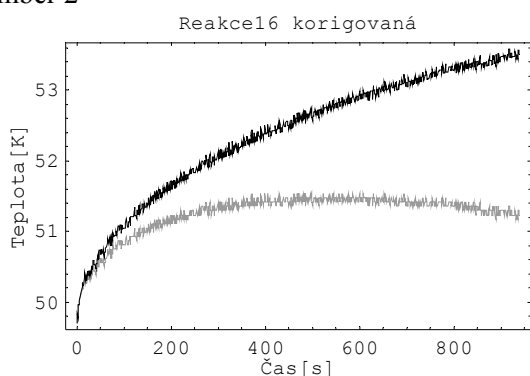


Fig. 9 Temperature course of the experiment number 3

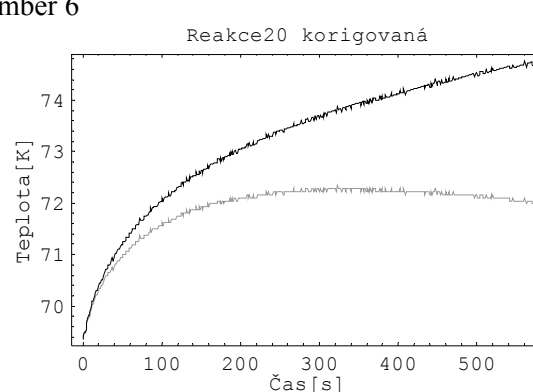


Fig. 13 Temperature course of the experiment number 7

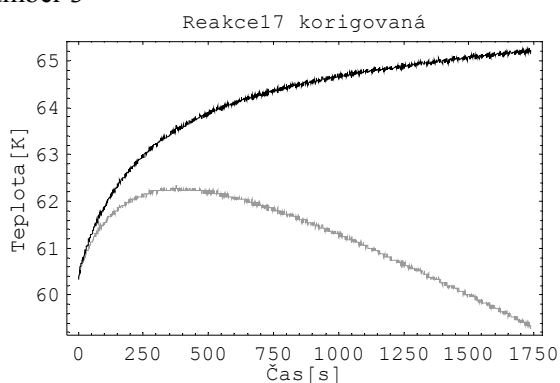


Fig. 10 Temperature course of the experiment number 4

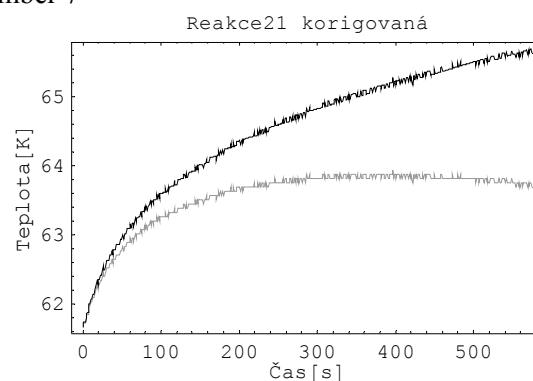


Fig. 14 Temperature course of the experiment number 8

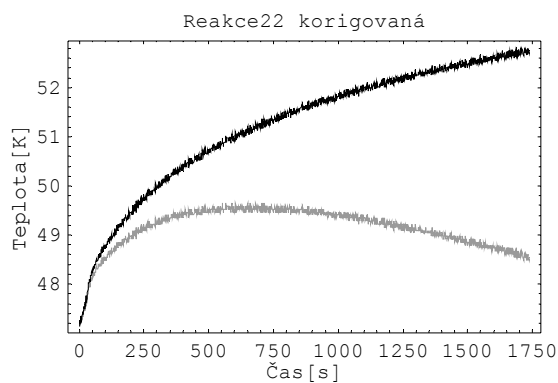


Fig. 15 Temperature course of the experiment number 9

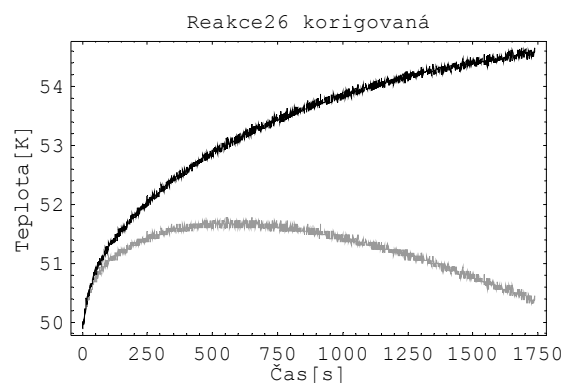


Fig. 19 Temperature course of the experiment number 13

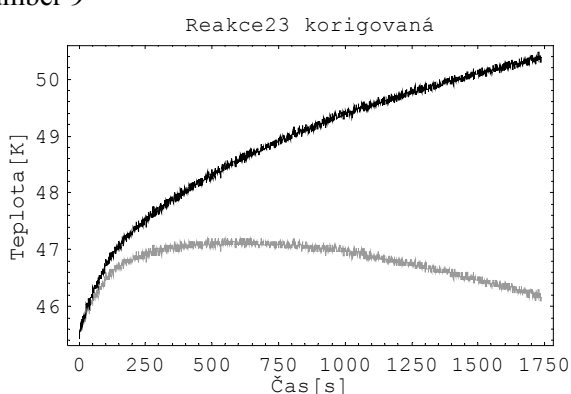


Fig. 16 Temperature course of the experiment number 10

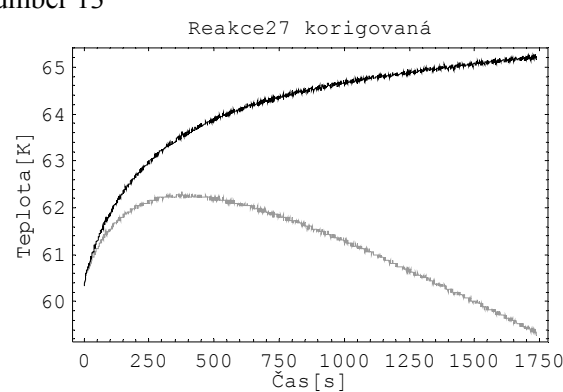


Fig. 20 Temperature course of the experiment number 14

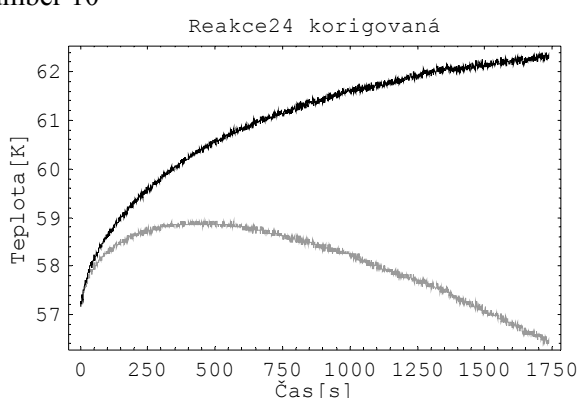


Fig. 17 Temperature course of the experiment number 11

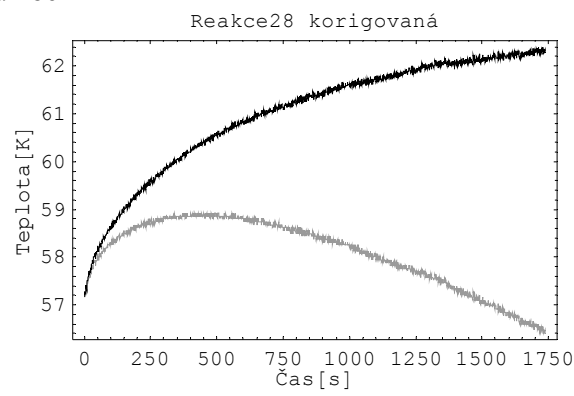


Fig. 21 Temperature course of the experiment number 15

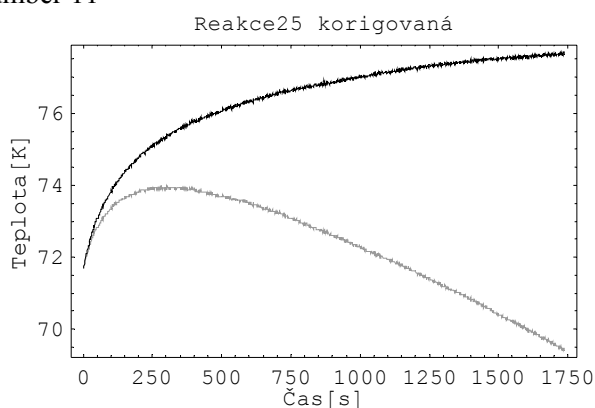


Fig. 18 Temperature course of the experiment number 12

Each of the graphs (7) to (21) contains two plots, the lighter (lower values) and darker (with higher values).

For the rate constants evaluating the darker sequences, which include correction for the heat loss by calorimeter wall, were used.

Table 2 Values of tangent directions obtained from the reactions temperature profiles

Number of experiment	Initial temperature $T_i$ [°C]	$y = fx + gx + h$			The value of reliability	Tangent direction
		f	g	h		
1	66.7	-0.00024215	0.15699	42.56	0.994	<b>0.0396793</b>
2	57.8	-0.00012886	0.04513	55.08	0.977	<b>0.0284066</b>
3	49.7	-0.00032659	0.10021	42.81	0.907	<b>0.0320855</b>
4	67.6	-0.00039859	0.09107	64.42	0.997	<b>0.0615223</b>
5	59.4	-0.00035777	0.08452	55.84	0.994	<b>0.0478254</b>
6	48.5	-0.0003534	0.12939	37.95	0.982	<b>0.0420451</b>
7	69.4	-0.00047559	0.11793	63.63	0.996	<b>0.0589316</b>
8	61.7	-0.00027607	0.12635	48.35	0.994	<b>0.0397258</b>
9	47.1	-0.00008266	0.42358	493.44	0.976	<b>0.0279079</b>
10	45.4	-0.00001619	0.07829	46.80	0.896	<b>0.0148859</b>
11	57.2	-0.00021315	0.82472	739.77	0.976	<b>0.0300658</b>
12	71.7	-0.00016737	0.51372	321.01	0.994	<b>0.0367624</b>
13	49.9	-0.00018025	0.02626	49.87	0.970	<b>0.0283253</b>
14	60.3	-0.00011829	0.39803	273.55	0.984	<b>0.0240583</b>
15	67.2	-0.00012745	0.32201	134.93	0.992	<b>0.0305415</b>

Table 3 Calculated values of rate constants

Number of experiment	Initial temperature $T_i$ [°C]	Heat capacity of calorimeter $C$ [J/K]	Number of moles of reactant $n$ [mol]	$\Delta H_r \cdot n$ [J]	Rate constant $k$ [1/s]
1	66.7	922.99	0.003557	6975.672	<b>0.0052502</b>
2	57.8	880.55	0.003557	6975.672	<b>0.0035858</b>
3	49.7	765.11	0.003557	6975.672	<b>0.0035192</b>
4	67.6	922.99	0.003571	7003.519	<b>0.008108</b>
5	59.4	880.55	0.003592	7045.289	<b>0.0059774</b>
6	48.5	765.11	0.003521	6906.054	<b>0.0046581</b>
7	69.4	922.99	0.003535	6933.901	<b>0.0078446</b>
8	61.7	880.55	0.003585	7031.366	<b>0.0049749</b>
9	47.1	765.11	0.003542	6947.825	<b>0.0030733</b>
10	45.4	765.11	0.003514	6892.131	<b>0.0016525</b>
11	57.2	880.55	0.003585	7031.366	<b>0.0037652</b>
12	71.7	922.99	0.003564	6989.595	<b>0.0048546</b>
13	49.9	765.11	0.003599	7059.213	<b>0.00307</b>
14	60.3	880.55	0.003542	6947.825	<b>0.0030491</b>
15	67.2	922.99	0.003606	7073.136	<b>0.0039855</b>

The values of polynomial coefficients for the individual experiments and their derivatives are listed in table 2.

The calculated values of rate constants for the individual experiments are than shown in table 3

Now we can use relation (13) and draw the dependence of  $\ln k$  on  $1/T$ . After fitting this

dependence by a straight line  $y = a + bx$ , we can determine the values of coefficients  $a$  and  $b$  and according to the formulas (14) and (15) calculate the value of pre-exponential factor  $A$  and activation energy  $E$ . The values of  $\ln k$  and  $1/T$  are shown in table 4. The  $1/T$  value in the table 4 is the reciprocal to the experiment initial temperature. A graphical



representation of the  $\ln k$  on  $1/T$  dependence is shown in figure 28.

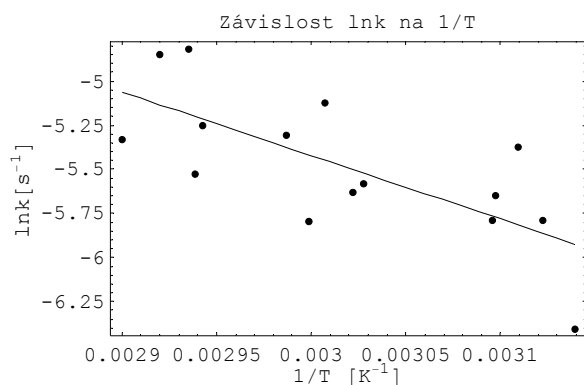


Fig. 28 Dependence of  $\ln k$  on  $1/T$

Based on the figure 7 the counted value of the coefficient  $a$  was  $-1.516$ , the value of  $b$  than  $-3604.4634$ . Substituting the relations (14) and (15) we obtain the relations (16) and (17), from which we determine the value of activation energy  $E$  and the pre-exponential factor  $A$ .

$$k_0 = e^a = e^{-1,5160} = 219,588 \text{ [s}^{-1}\text{]} \quad (16)$$

$$E = -bR = -(-3604,4634 * 8,314) = 29967,5087 \text{ [J.mol}^{-1}\text{]} \quad (17)$$

After substituting into equation (5) is the resulting expression for the rate constant given by (18):

$$k = k_0 e^{-\frac{E}{RT}} = 219,588 e^{-\frac{3604,4634}{T}} \quad (18)$$

## 5 Conclusion

The semi-batch exothermic reactor control is a complex and difficult process. One of the difficulties is the changing reaction rate which is causing the system nonlinearity as is shown in this paper. However it is possible to deal with the problem by the rate constant identification based on the temperature profile. With the help of the formula (6) we can use an in-reactor temperature profile to find the rate constant directly from the process (in case we put known chemicals quantity in the reactor). The chemicals volume and the starting concentration are usually known. The system (reactor) thermal capacity must be determined, but only once. Finally the temperature tangent direction may be obtained from the measured temperature time dependence.

The whole procedure had been already verified by author during the chromium sludge processing [6].

Table 4 Values of  $\ln k$  and  $1/T$

Number of experiment	Initial temperature $T_I$ [°C]	Rate constant $k$ [1/s]	$\ln k$ [1/s]	$1/T$ [1/K]
1	66.7	0.0052502	<b>-5,249</b>	<b>0,002942</b>
2	57.8	0.0035858	<b>-5,631</b>	<b>0,003022</b>
3	49.7	0.0035192	<b>-5,650</b>	<b>0,003097</b>
4	67.6	0.008108	<b>-4,815</b>	<b>0,002935</b>
5	59.4	0.0059774	<b>-5,120</b>	<b>0,003007</b>
6	48.5	0.0046581	<b>-5,369</b>	<b>0,003109</b>
7	69.4	0.0078446	<b>-4,848</b>	<b>0,002920</b>
8	61.7	0.0049749	<b>-5,303</b>	<b>0,002987</b>
9	47.1	<b>0.0030733</b>	<b>-5,785</b>	<b>0,003122</b>
10	45.4	<b>0.0016525</b>	<b>-6,405</b>	<b>0,003139</b>
11	57.2	<b>0.0037652</b>	<b>-5,582</b>	<b>0,003028</b>
12	71.7	<b>0.0048546</b>	<b>-5,328</b>	<b>0,002900</b>
13	49.9	<b>0.00307</b>	<b>-5,786</b>	<b>0,003096</b>
14	60.3	<b>0.0030491</b>	<b>-5,793</b>	<b>0,002999</b>
15	67.2	<b>0.0039855</b>	<b>-5,525</b>	<b>0,002938</b>

The rate constant knowledge can help us to set up a precise system model and to apply a suitable control method. With a system model even simple control methods can be used to control some specific batch reactors. On the above mentioned system some control methods had been applied, which were described in articles [7,8,9,10]. Very powerful seems to be for example predictive control using neural networks [7].

Although this article deals with semi-batch processes, the influence of reaction kinetics can be found also in other processes. For example mathematical models of continuous stirred tank reactor also contain Arrhenius equation [11,12,13], or alternatively the batch reactor described in [14] as well. The described method could be possibly used in those cases too.

## 6 Acknowledgement

This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic under grant MSM 7088352102. This support is gratefully acknowledged.

### References:

- [1] Luyben, W. L., Fed-Batch Reactor Temperature Control Using Lag Compensation and Gain Scheduling, *Industrial & Engineering Chemistry Research*, Vol. 43, 2004, pp. 4243-4252.
- [2] Bouhenchir, H., Cabassud, M., Le Lann, M V., Predictive functional control for the temperature control of a chemical batch reactor, *Computers and Chemical Engineering*, Vol. 30, 2006, pp. 1141-1154.
- [3] Kolomazník, K., Adámek, M., Uhlířová, M., Potential Danger of Chromium Tanned Wastes, In *Proceedings of the 5th IASME/WSEAS International Conference on Heat Transfer, Thermal Engineering and Environment*, IASME/WSEAS, 2007, pp. 137-141.
- [4] Janacova, D., Kolomazník, K., Mokrejs, P., Vasek, V., Optimization of enzymatic hydrolysis of leather waste, In *Proceedings of the 6th WSEAS International Conference on Applied Informatics and Communications*, WSEAS, 2006, pp. 345-348.
- [5] Macků, L., Sámek, D., Two step, PID and model predictive control using artificial neural network applied on semi-batch reactor, *WSEAS Transactions on Systems*, Vol. 9, No. 1, 2010, pp. 1039-1049, ISSN 1109-2777.
- [6] Macků, L., *Control design for the preparation of regenerate for tanning*, Ph.D. Thesis, UTB in Zlín, 2003.
- [7] 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, 2007, pp. 180-185.
- [8] Gazdoš, F., Macků, L., Analysis of a semi-batch reactor for control purposes, In *Proceedings of 22nd European Conference on Modelling and Simulation ECMS 2008*. Nicosia, Cyprus, 2008, pp. 512-518, ISBN 978-0-9553018-5-8.
- [9] Novosad, D., Macku, L., Ziegler-Nichols controller with online identification versus PID controller comparison, In *Annals of DAAAM for 2010 & Proceedings of the 21st International DAAAM Symposium*, 2010, pp 1017-1018, ISBN 978-3-901509-73-5, ISSN 1726-9679.
- [10] Novosad, D., Macku, L., Pole placement controller with compensator adapted to semi-batch reactor process, In *Proceedings of 13th WSEAS International Conference on AUTOMATIC CONTROL, MODELLING & SIMULATION (ACMOS '11)*, 2011, pp. 341-345, ISBN: 978-1-61804-004-6.
- [11] Dostál, P., Gazdoš, F, Bobál, V., Bakošová, M., Nonlinear Adaptive Control of a Chemical Reactor, In *Proceedings of 13th WSEAS International Conference on AUTOMATIC CONTROL, MODELLING & SIMULATION (ACMOS '11)*, 2011, pp. 45-50, ISBN: 978-1-61804-004-6.
- [12] Bahmanpour, S. , Bashooki, M., Refan, M., H., State Estimation And Fault Diagnosis Of Industrial Process By Using of Particle Filters, In *Proceedings of the 6th WSEAS International Conference on Signal Processing, Robotics and Automation*, 2007, pp. 208-213, ISBN: 978-960-8457-59-1
- [13] Hourfar, F., Salahshoor, K., Paivar, A., A Neural Adaptive Feedback Linearization Control for CSTR Using NARMA-L2 Model, In *Proceedings of the 5th WSEAS Int. Conf. on CIRCUITS, SYSTEMS, ELECTRONICS, CONTROL & SIGNAL PROCESSING*, 2006, pp. 285-290, ISBN: 960-8457-55-6
- [14] Thitiyasook, P., Kittisupkorn, P., Model Predictive Control of a Batch Reactor with Membrane-based Separation, In *Proceedings of the 7th WSEAS International Conference on SIGNAL PROCESSING, ROBOTICS and AUTOMATION (ISPRA '08)*, 2008, pp. 88-92, ISBN: 978-960-6766-44-2.