A FEEDBACK TEMPERATURE CONTROL IN A CHEMICAL REACTOR WITH HIGH INERTIA OF ITS COOLING SYSTEM

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In this work we compare simple algorithms for the on—off feedback temperature control of the reaction mixture in a batch reactor during an exothermic reaction. The aim of the control was to maintain the temperature of the mixture within the given range and, simultaneously, to minimize the number of the regulator switchings. The temperature control of the mixture was being performed at conditions when working states of the reactor in an open regulation loop are unstable and when the response of the cooler to regulation is slow. The following control algorithms were compared: P — regulator, PD — regulator and algorithms based on a prediction mathematical model including its adaptive variant. The results indicate that the algorithms based on the mathematical model are more efficient. However, the precision of the control can be diminished due to error in the time derivative of the temperature of the reaction mixture which forms the input to the prediction model. The adaptive variant of the algorithms was advantageous in cases when it was necessary to make up for significant errors in initial estimates of parameters of the prediction mathematical model.

During the automation of smaller chemical plants it is sometimes necessary to solve the problem of temperature control in a reactor whose dynamic properties are unsuitable due to a high inertia of its cooling system. Reactors cooled by a voluminous cooling jacket may serve as an example. The inappropriate construction (large volume) of the jacket slows down the effect of the cooling system. Pressure reactors (autoclaves), where the inertia of their cooling system is brought about by the large mass of the reactor wall, form another such example.

It is the aim of this work to verify on a laboratory model equipment whether it is possible to control reliably the temperature of the reaction mixture with a feedback regulator in a reactor with unfavourable dynamic properties also when its working state is unstable at the open regulation loop. Here we compare the effectiveness of the classical temperature control algorithm (PD) which is based on the "black box" concept, with a control system using a predictive simulation model of the system. We also verified some adaptive variants of the algorithm based on the mathematical model of the reactor.

EXPERIMENTAL

The principle and aim of the reaction temperature control. We controlled the temperature of the mixture with an on-off regulator. The active part was formed by a moving cooler, whose heat-transfer surface could be varied. This device has been described in our earlier work[1] and its schema is in Fig. 1. The batch reactor is isolated from its surrounding and the reaction heat is taken off by a cylindrical cooler which is submerging or emerging out of the reaction mixture at a constant rate. Thus, the rate of cooling of the reaction mixture is determined by the instantaneous magnitude of the transfer surface (the submerged part of the cooler). The rate of motion of the cooler can be varied within the range of three orders of magnitude which enables to change dynamic properties of the cooling system at otherwise constant properties of the system. The motion of the cooler is controlled by the control algorithm. In the first position of the regulator, the cooler is moving downwards or it remains in one of the extreme positions (it is entirely submerged). In the second position, it is emerging from the reaction mixture or it remains in the other extreme position (it is entirely emerged).

The aim of the control was to maintain the temperature of the reaction mixture within the given range $T_s \pm \Delta T_{reg}$ and to minimize simultaneously the number of switchings of the regulator (changes in the direction of motion of the cooler). These requirements are fulfilled just when the temperature of the reaction mixture is oscillating around the given value so that it is just reaching the maximum permissible deviations from this value (it oscillates between the two bounds of the temperature range).

Reaction conditions and characteristic parameters of the rate equation for the model reaction have also been described in our earlier work published in this journal[1].

As the regulator we employed a digital computer (Video Genie System EG 3003) communicating with the control system in an off-line manner. The beginning of the experiment was identical in all cases. The cooler was at the beginning set up so that its transfer surface might assume the value corresponding to the pseudostationary state of the reactor ($P_s = 0{\cdot}926 \cdot 10^{-3}\ \mathrm{m}^2$). The reaction was initiated by addition of a catalyst at 337 K and, as soon as the temperature of the mixture reached the value of 339 K, the given algorithm started to control the system. The algorithms compared were verified experimentally at conditions when the rate of motion of the cooler was low. The time, during which the cooler passes from one extreme position to the other, was

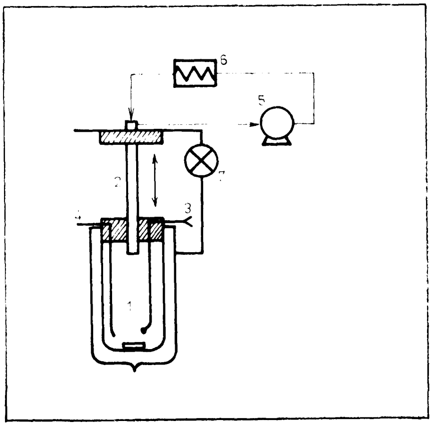

FIG. 1

The scheme of the laboratory equipment (controlled system). **1** reactor (Dewar vessel), **2** cooler, **3** thermocouple, **4** resistance heating for compensation of heat losses to the surroundings, **5** pump, **6** thermostat, **7** motor and mechanism conveying the cooler

$t_c = 1\,684$ s. The following quantity was employed to characterize the inertia of the cooling system. If the reaction proceeded adiabatically, the temperature would grow at the required temperature by the rate described by the equation

$$\frac{dT}{dt} = \frac{r(-\Delta H)}{\varrho c_p} . \tag{1}$$

At this rate, the temperature would change by the interval equal to $2\,\Delta T_{reg}$ after the time determined by the relation

$$\Delta t_{ad} = \frac{2\,\Delta T_{reg}}{dT/dt} = \frac{2\,\Delta T_{reg} c_p \varrho}{r(-\Delta H)} . \tag{2}$$

After the time Δt_{ad}, the rate of cooling will change, relatively to the value corresponding to the pseudostationary state, by the value determined by the relation

$$\frac{\Delta A}{A_s} = \frac{A_{max}}{A_s t_c} \Delta t_{ad} . \tag{3}$$

Both the time Δt_{ad} and the relative change of the rate of cooling depend on the degree of conversion. The values are given in Table I.

The sampling of temperature. For the purpose of the digital processing, the deviation in the reaction temperature was divided into equidistant levels differing by 0·1 K. The time at which the temperature reached a given level was taken as the input. In this manner we employed in the processing only those points which are equidistant from the point of view of the reaction temperature. From these data we determined the value of the temperature derivative with respect to time. As soon as the temperature reached some of the discrete levels, the control algorithm decided whether to perform the switching or to preserve the existing state of motion of the cooler.

Algorithm of Control

The PD-*algorithm.* The condition for the switching was determined from the equation

$$A_v = T - T_s + D_k(dT/dt) . \tag{4}$$

TABLE I

The effect of the degree of conversion of hydrogen peroxide, x, on the magnitude of the relative change of the heat transfer area after time Δt_{ad} at temperature $T_s = 339$ K

x	0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8
Δt_{ad}, s	145·36	169·36	166·27	151·21	157·97	183·77	238·89	358·86	683·8
A/As	0·130	0·177	0·171	0·141	0·154	0·208	0·352	0·795	2·888

The cooler is moving upwards for $A_v \leqq 0$ and downwards for $A_v \geqq 0$. The quantity D_k is the dynamic gain of the regulator and it is only adjustable parameter.

The non-simplified prediction reactor model (*model* I). As soon as the temperature reached some of the levels, the further course of the temperature was predicted by simulation. This prediction was calculated from the model based on the balance of the key component.

$$\frac{dx}{dt} = \frac{r}{c_{B0}} = k_0 f(x) \exp \frac{E}{RTT_0} (T - T_0) \tag{5}$$

on the heat balance

$$\frac{dT}{dt} = \frac{T_{ad} r}{c_{B0}} - A(T - T_{ci}) \tag{6}$$

and on the description of the rate of changes of the position of the cooler

$$\frac{dA}{dt} = \pm \frac{A_{max}}{t_c} . \tag{7}$$

Initial conditions for the numerical integration were determined in the following manner:
The temperature corresponds to the reached level ($T = T_n$). The degree of conversion was not determined experimentally by analyzing the mixture, but from computations — by subsequent integration of the model (Eq. (*5*)) from the beginning of the reaction up to the given moment. Nor the instantenuous position of the cooler, the quantity A, was determined from measurements, but by computations from the model

$$A_0 = (dT/dt - T_{ad} r/c_{B0})/(T_{ci} - T) . \tag{8}$$

The dependence of the reaction rate on the degree of conversion of the key component was described within the range of the degree of conversion as

$$x \in (0; 0{\cdot}15)\, f(x) = 1 - 1{\cdot}4171x , \tag{9}$$

$$x \in (0{\cdot}15; 1{\cdot}0)\, f(x) = (1 - x)^{1.87} x^{0.85} . \tag{10}$$

The activation energy of the model reaction is 90 kJ mol_B^{-1}. The direction of motion of the cooler was changed when the prediction indicated that the admissible tolerance ΔT_{reg} would be exceeded if the direction of motion of the cooler remained unchanged (Fig. 2).

The linearized prediction model (model II). It is assumed in this model that it is possible to neglect the effect of changes in the degree of conversion and the temperature on the reaction rate during the switching cycle. In the computations we employed the constant value of the reaction rate corresponding to the preceding switching cycle.

The adaptive prediction model (model III). In this algorithm of control, the value of k_0 in Eq. (*5*) is adjusted on the basis of a comparison between the prediction and the actual course of the temperature after the switching of the direction of the motion of the cooler has been performed. The value of constant k_0 was being adjusted so that the non-simplified model might agree with the measured value. The new value was then employed to control the temperature in the following cycle.

The evaluation of k_0 was based on comparison of the observed and calculated overregulation of the reaction temperature.

RESULTS AND DISCUSSION

THE EFFECT OF NOISE IN THE TEMPERATURE MEASUREMENT ON THE ACCURACY OF THE TEMPERATURE CONTROL OF THE REACTION MIXTURE

Both the measurements and simulation calculations were performed in the working state of the reactor which is "strongly" unstable at the open regulation loop. In this case we must use for controlling the reaction temperature in the reaction mixture such an algorithm which can predict the behaviour of the controlled system. The fact that the working state of the reactor is unstable was proven by the course of the temperature if it is controlled by the PD algorithm with a zero gain $D_k = 0$. This algorithm corresponds to a simple relay and it does not contain any prediction term. The result see Fig. 3, curve *1*. The control using this algorithm failed.

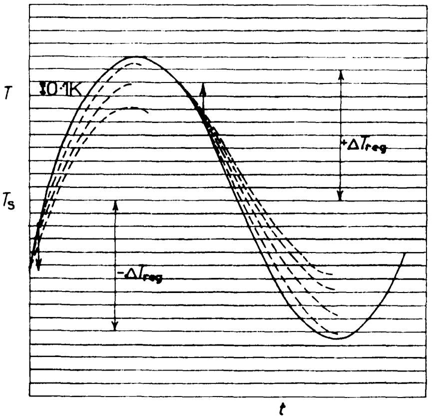

FIG. 2

The scheme of the process of prediction of the reaction temperature course with the help of the mathematical model of the system. Full line — actual temperature course (T), dashed line — predicted temperature course (T_{sim}). The arrows mark moments of the regulation action (↓ switching leading to submersion, ↑ switching leading to emergence)

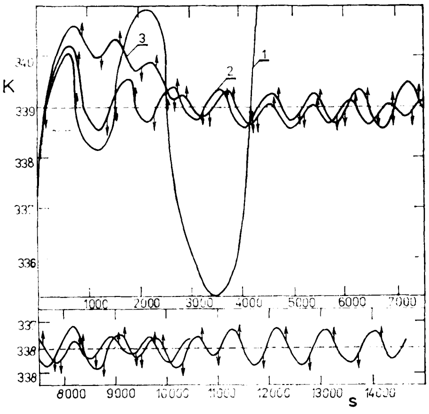

FIG. 3

Examples of the time dependence of the reaction temperature for experimental tunings of the PD regulator (The effect of the amplification of the derivative gain component, D_k). *1* $D_k = 0$ (ideal relay), *2* $D_k = 100$ s, *3* $D_k = 1\ 000$ s

The prediction model requires as the input information not only the instantaneous temperature of the reaction mixture, but also the rate of its changes. This quantity was described by the instantenuous value of the time derivative of temperature. Results of our investigations showed that if the reaction temperature is controlled by on-off regulators, it is the determination of the temperature derivative which forms the source of uncertainty. It is due to two reasons. Any determination of a derivvative is generally affected by noise more than a determination of the deviation from the required value. With an on-off control, the temperature moreover oscillates around the given value. Consequently, changes in the derivative are rapid and significant, which diminishes the possibility of using efficient filtration methods for experimental data. A data filtration of an oscillating quantity can be namely performed only if the basis of this filtration is a time interval smaller than 1/4 of the vibration period. If the filtration extends over a larger time interval, it is simultaneously damping the sensitivity of following the state of the system. We must consider this fact if we compare the effectiveness of the individual algorithms. Thus, inaccuracies in the determination of the temperature derivative set limits to a perfect control. Even if we employ the "absolutely accurate" prediction model, the accuracy of the temperature control cannot be higher than the corresponding accuracy of the temperature derivative. An example of the effect of the inaccuracy in the determination of the derivative on the magnitude of the temperature overregulation is given in Table II. For an assumed noise bandwidth $\Delta T_n = 0{\cdot}01$ K and the sampling interval $\Delta T = 20$ s, we obtain $\Delta D_r = 2\,\Delta T_n/\Delta t = 0{\cdot}001$ K s^{-1}.

The aim of the control was to make the reaction temperature oscillate around a given value with the deviation just equal to the maximum allowed regulation deviation, $\Delta T_{reg} = 1$ K. It follows from our analysis of the effect of noise on the

TABLE II

The effect of the noise bandwidth in the time derivative of the reaction temperature on the temperature course. 1: $x = 0{\cdot}127$, $A_0 = 1{\cdot}204 \,.\, 10^{-4}$ s^{-1}, $D_r = 5 \,.\, 10^{-3}$ Ks^{-1}; 2: $x = 0{\cdot}519$, $A_0 = 1{\cdot}169 \,.\, 10^{-4}$ s^{-1}, $D_r = 4{\cdot}17 \,.\, 10^{-3}$ Ks^{-1}. Initial conditions 1 and 2 were obtained experimentally (Fig. 4) for $\Delta T_{reg} = 1$ K

1			2		
δ_{Dr}, %	$A_0 \,.\, 10^{-4}$, s^{-1}	ΔT_{ext}, K	δ_{Dr}, %	$A_0 \,.\, 10^{-4}$, s^{-1}	ΔT_{ext}, K
20	1·013	0·37	23·9	0·979	0·29
20	1·394	−0·27	23·9	1·360	−0·23

derivative that not even the most perfect algorithm of control can fulfil the aim of the control with a smaller error than 0·3 K. If we increase the maximum allowed temperature deviation, the effect of an error in the determination of the derivative also increases since both the value of the derivative itself and the rate of its changes (the second derivative) increase with increasing the oscillation range.

The PD *Regulator*

This type of regulator was developed for the control of linear systems with constant properties and it does not enable to include a more complex information about the process into the algorithm. The only parameter in this regulator is, at a given value of the reaction temperature, the gain of the differential component, D_k, in the equation of the regulator (relation (*4*)). The determination of the optimum value of this amplification is usually denoted as a "regulator tuning". An example of the regulator tuning by trial and error is in Fig. 3. During the control in an unstable state, values of the gain are bounded from both directions[2-4]. In accordance with our earlier results[1] we found out that the gain interval is extremely narrow. A PD regulator is not of course able to tackle changes in the system properties arising during the process such as, *e.g.*, changes in the reaction rate, heat output, *etc.*

Prediction Algorithms Based on a Mathematical Model of the Controlled System

An advantage of prediction models based on a mathematical model consist in the fact that they enable to include into the algorithm of control the information about the system obtained during the development of the process and during the design: they can be, for example, the effects of temperature or of the degree of conversion on the reaction rate, *etc.* As long as we have at our disposal a model of the equipment, the problem of the regulator tuning disappears, since the algorithm is able to find values of switching points only from requirements imposed on the quality of the control. Examples illustrating the ability of the algorithm to respond to given requirements are given in Figs 4 and 5, where temperature courses of the reaction mixture for two given maximum permissible deviations $\Delta T_{reg} = 1$ K and 2 K are compared. The result proves that the algorithm based on the deterministic model of control is able to fulfil the task semiquantitatively. However, this result is strongly affected by the error in the derivative.

We used two nonadaptive mathematical models to predict the behaviour of the reactor, namely the linearized model (model II) and the non-simplified mathematical model (model I). The comparison between temperature courses of the reaction mixture as controlled by these two algorithms is in Figs 4 and 5. Approximately we may say that the difference between the more precise and the simpler algorithm almost disappears due to the error in the determination of the temperature derivative.

The more precise prediction model (I) employs a more accurate value of the degree of conversion. The degree of conversion of hydrogen peroxide was not determined experimentally, but by computation. In the simplified model (II), the degree of conversion is determined with an error which increases gradually and thus it loads the model with a systematic error. As in our studies a very slow computer was used for on line simultations the efficiency of the more sophisticated model was reduced by the delay of the control action due to increase in the time necessary for simulations.

The Effect of Inaccuracies in Input Data to the Model on the Accuracy of the Control

In a real plant, we shall have to take into account that the input composition, the catalyst activity or the quality of exchangeable plates may vary. To test the resistance of the algorithms with respect to errors in parameters of the model, we performed several series of measurements containing an error in the input value of the reactivity. The results are in Figs 6 and 7. The most dangerous case arises when the actual reactivity is higher than the model one. Since the reaction rate increases with increasing temperature, the model with the lower value underestimates heat effects

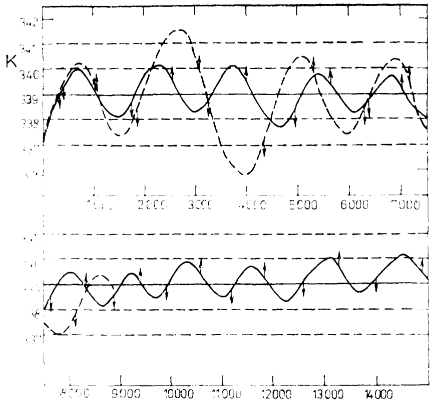

FIG. 4

The experimental verification of the ability of the algorithm to respond to the maximum admissible deviation in the reaction temperature, ΔT_{reg}. Model II; full line — course of the reaction temperature for $\Delta T_{reg} = 1$ K, dashed line — $\Delta T_{reg} = 2$ K.

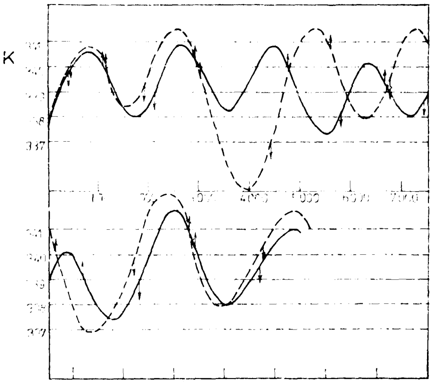

FIG. 5

The experimental verification of the ability of the algorithm to respond to the maximum admissible deviation in the reaction temperature, ΔT_{reg}. Model I; for the notation see Fig. 4

of the reaction. It is apparent that small deviations (*e.g.*, 10%) cannot cause a failure, larger deviations (50%) either deteriorate substantially the quality of the control or they lead to a failure.

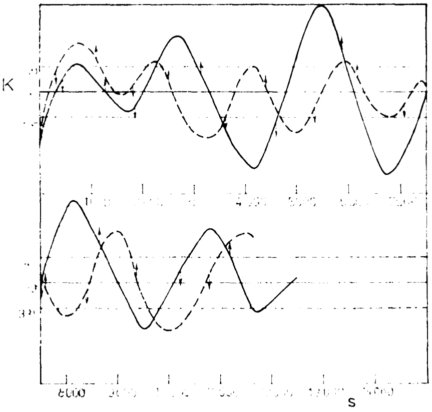

FIG. 6

The experimental verification of the resistance of nonadaptive algorithms tested to the error in input parameters of the prediction model (increase in the catalyst concentration in the experiments performed by 10%). Dashed line — regulation by model I, full line — regulation by model II

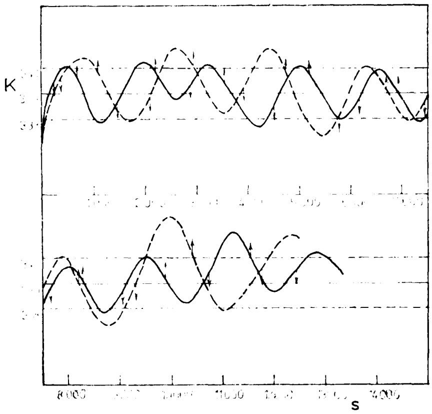

FIG. 7

The comparison of the reaction temperature control with the help of the adaptive and the nonadaptive algorithm (with the identical model reactivity). Dashed line — regulation by model II, full line — regulation by model III

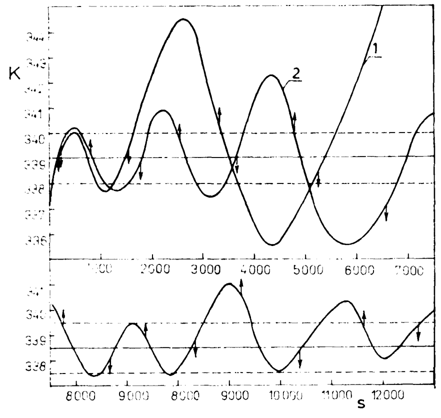

FIG. 8

Experimental verification of the resistance of the nonadaptive and the adaptive algorithm to an 50% decrease in the reactivity of the prediction model. **1** regulation by model I, **2** regulation by model III

Adaptive Algorithm (model III)

The simple adaptive algorithm employed enables to adjust values of the reactivity of the mixture from a comparison between the predicted and the actual temperature course. We compare the magnitude of the over-regulation, *i.e.*, the magnitude of the largest deviation between the predicted and the actual temperature. The adaptivity of the model is total, which means that the value of the reactivity in the model is replaced with a new one based on a single last comparison of the deviations. Consequently, the effect of the error in the determination of the temperature derivative will be fully included in the new value of the reactivity. Thus, the application of this algorithm cannot offer a substantially more accurate temperature control than that corresponding to the error in the derivative. Fig. 7 contains a comparison between temperature controls of the reaction mixture with the help of the adaptive and the nonadaptive model, resp. The adaptive model becomes an effective improvement only if the input model is loaded with a high error. Such an example is in Fig. 8. The use of the nonadaptive model with an erroneous input value of the reactivity (it was ~50% of the correct value) was followed by a failure, however, the adaptive model gave an acceptable quality of the control.

LIST OF SYMBOLS

$A = khP/Vc_p$	parameter in the balance equation (*6*) (s^{-1})
A_0	value of the parameter A at the moment of the control action (s^{-1})
A_{max}	maximum value of A corresponding to the full submersion of the cooler (s^{-1})
A_s	value of A corresponding to the pseudostationary state (s^{-1})
A_v	action quantity (K)
c_{Bo}	initial concentration of hydrogen peroxide ($kmol\,m^{-3}$)
c_p	specific heat of the reaction mixture ($J\,K^{-1}\,kg^{-1}$)
D_k	derivative gain of the PD regulator (s)
E	activation energy ($J\,mol^{-1}$)
$f(x)$	functional relation for the dependence of the reaction rate on the degree of conversion of hydrogen peroxide
ΔH	enthalpy of reaction ($J\,mol_B^{-1}$)
k_0	constants in rate equations (ref.[1]) (s^{-1})
k_h	heat transfer coefficient ($W\,K^{-1}\,m^{-2}$)
P	heat transfer area (m^2)
R	gas constant ($J\,mol^{-1}\,K^{-1}$)
r	reaction rate ($kmol_B\,m^{-3}\,s^{-1}$)
T	temperature of the reaction mixture (K)
T_{ad}	adiabatic temperature rise (K)
T_{ci}	temperature of the heat transfer medium (K)
T_{ext}	temperature at the extreme point (maximum or minimum) for the course with a given error D_r in the determination of the derivative
$(T_{ext})_p$	temperature at the extreme point for the course with the value of the derivative corresponding to the experiment being compared
T_s	required temperature of the reaction mixture (K)

ΔT_{reg}	permitted overregulation of the temperature of the mixture (K)
$\Delta T_{ext} = T_{ext} - (T_{ext})_p$	
t	time
V	volume of the reactor (m^3)
x	degree of conversion of hydrogen peroxide
ϱ	specific mass of the reaction mixture
$\delta Dr = \Delta Dr/Dr$	relative error in the determination of the derivative
Dr	calculated time derivative of the temperature
ΔDr	error in the determination of the derivative

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