A TWO-POINT REGULATOR CONTROL OF A CHEMICAL REACTOR; COOLING SYSTEM WITH A LARGE INERTIA — PD ALGORITHM

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The effect has been investigated of the gain of the derivative element of a PD controller on the quality of the temperature control of an exothermal reaction mixture in a batch reactor. The investigation concerned a reactor equipped with a cooling system whose rate of response could be varied in the range of several orders of magnitude. The results have lead to the conclusion that a slow response of the cooling system is difficult to make up for by using more sophisticated control algorithms. For the slow response of the cooling system the range of gain of the controller providing for a safe temperature control is narrow leaving essentially no margin for its practical utilization. The study combined simulation on a mathematical model with experimental verification of a laboratory scale reactor cooled by a submersible retractable cooler.

Temperature control of chemical reactors whose cooling systems respond quickly to a change of the manipulated variable, *e.g.* the flow rate of the coolant, can be accomplished by simple means even with the aid of the simplest control algorithms. The control is simple and reliable even if the reactor operates in an unstable steady state[1,2]. If the response of the cooling systems is sluggish, difficulties arise and more sophisticated forms with a predictive feature, such as *e.g.* the proportional — plus — derivative (PD) algorithms must be used.

Control of large reactors with an unfavourable ratio of the extent of the cooling surface to volume necessitates utilization of also operational points which are open-loop unstable. Temperature control of the reaction mixture in such reactors requires feed back control for even a simple stabilization of inlet streams does not suffice for maintaining the temperature at a requested level. For the control in an unstable point the problem of tuning a PD regulator is different from that in a stable point. In the stable state it is desirable to achieve maximum gain of the derivative component of the controller as the quality of the control improves with increasing gain. The maximum gain is limited by stability of the closed-loop. At high gains the control loop becomes unstable and oscillates.

Control in an unstable point is limited by both the maximum and the minimum gain. The minimum gain is set by the requirements on stability of the control loop. For small gains the loop is unstable and the regime drifts into the undesirable stable point. From the standpoint of stability it is therefore advantageous to work with high gains. High gain, however, simultaneously amplifies the effects of nonidealities of the loop (lagging of detectors, actuators, noise) which results in impaired quality of the control and eventuality instabilities[3-6].

The aim of this work has been to study the effect of the gain of the derivative element of the PD regulator on the quality of the temperature control of an exothermal reaction in a batch reactor in dependence on the rate of response of the cooling system.

EXPERIMENTAL

Description of the reactor. The measurements were carried out in a laboratory mixed batch reactor (Dewar vessel) of volume $5{\cdot}6 \cdot 10^{-4}$ m^3 ref.s[7,8]. In the reactor there was a resistance electric heater whose thermal input compensated for the losses of heat to the surroundings. The heat of reaction was removed from the reactor by a submersible retractable cylindrical cooler $4{\cdot}23 \cdot 10^{-6}$ m^3 in volume with $1{\cdot}75 \cdot 10^{-3}$ m^2 of heat transfer area. The flow rate of the coolant through the cooler was $6{\cdot}4 \cdot 10^{-6}$ m^3 s^{-1}. The inlet temperature of the coolant was 286 K. The experimentally determined heat transfer coefficient was 542 W m^{-2} K^{-1}. During the experiments the cooler moved down to be immersed into the reaction mixture of upward to be retracted from the reaction mixture. This altered the extent of the heat exchange surface available for cooling. The speed of motion of the cooler could be altered stepwise within three orders of magnitude (the traverse time from one extreme position to another was between 4·8 and 3503 seconds).

The temperature in the reactor was measured by copper-constantan thermocouple with a time constant 2 s. A digital computer Video Genie System LG 3003 was used for the control.

The model reaction. A strongly exothermic oxidation of ethanol by hydrogen peroxide catalyzed homogeneously by Fe(III) ions was used as a model reaction (reaction enthalpy −275 kJ . mol^{-1} of hydrogen peroxide). As has been found in the previous work[9], under the given reaction conditions the reaction exhibits autocatalytic properties. The following rate equation was used to described the course of the reaction

$$r/c_{A0} = k\, f(x) \exp\left(-10\,817{\cdot}5/(T)\right). \tag{1}$$

Functional dependence of the reaction rate on the degree of conversion of hydrogen peroxide in the range of conversion between 0·00 and 0·15 was taken in the form

$$k\, f(x) = 7{\cdot}9\,615 \cdot 10^9(1 - 1{\cdot}4171x) \tag{2}$$

and for higher conversions in the form

$$k\, f(x) = 4{\cdot}14925 \cdot 10^{10}(1 - x)^{1{,}87}x^{0{,}85}. \tag{3}$$

In all experiments the initial concentrations were: 1·941 kmol m^{-3} (hydrogen peroxide), 0·83 kmol m^{-3} (ethanol) and $5{\cdot}72 \cdot 10^{-4}$ kmol m^{-3} (catalyst).

The control algorithm. The temperature control of the reaction mixture was realized by a two-point controller. In one position of the controller the cooler moved down into the reaction mixture or remained in the extreme position (totally submerged). In the second position the cooler moved out of the reaction mixture or remained in the extreme position (totally retracted.) The direction of motion was determined by the algorithms of relay with hysteresis (temperature difference switch-over relay), the idetal relay (P regulator)[7,8], or PD algorithm.

Under the control following the relay with hysteresis algorithm the cooling of the reactor is actuated (the cooler is being submerged) provided the following condition is met

$$T \geqq T_s + T_{reg} \tag{4a}$$

or

$$dT/dt < 0 \quad \text{and} \quad T > T_s - T_{reg}. \tag{4b}$$

The cooling is terminated (the cooler is being retracte) provided the following condition is met

$$T \leqq T_s - T_{reg} \tag{5a}$$

or

$$dT/dt > 0 \quad \text{and} \quad T > T_s - T_{reg}\,. \tag{5b}$$

The temperature difference T_{reg} must be chosen greater than the band noise in the measured temperature. In case of the ideal relay algorithm the temperature difference T_{reg} is zero.

In case of the control following the PD algorithm the equation of the regulator takes the form

$$A_v = T - T_s + D_k(dT/dt)\,. \tag{6}$$

The cooling of the reactor is off provided that

$$A_v \geqq A_n\,, \tag{7}$$

where A_n is a value of the action variable corresponding to the given noise in the measured temperature of the reaction mixture

$$A_n \approx \Delta T_n(1 + 2(D_k/\Delta t))\,. \tag{8}$$

The cooling is off provided the following condition is met

$$A_v \leqq -A_n\,. \tag{9}$$

In the range of the action variable $A_v \in (A_n; -A_n)$ prevailing regulation status remains in effect.

Data acvuisition and derivative evaluation. Processing of the data on the course of the temperature of the reaction mixture was based on measurement of the time periods within which the temperature reached values $T_s \pm i\,.\,\Delta T_s$, where i is an integer. The interval ΔT_s was taken 0·1 K. The derivative was evaluated from the relation

$$dT/dt \approx \Delta T_s/\Delta t\,, \tag{10}$$

where Δt is the time during which the temperature changed from a level i to i + 1 or i − 1.

The noise band in the measurement of temperature estimated from the evaluated experimental temperatures of the reaction mixture was $T_n \approx 0.01$ K. Within the band $T_s \pm \Delta T_n$ it is thus impossible to distinguish whether the temperature is higher or lower than the requested temperature. Corresponding maximum error of the derivative of the temperature with respect to time then amounts to $\pm 2(\Delta T_n/\Delta t)$.

RESULTS AND DISCUSSION

The temperature control. Let us assume that the temperature of the reaction mixture in the reactor is to be maintained within a certain temperature interval $T_s \pm T_{reg}$ and, at the same time, the number of switchings of the regulator is to be minimized. This is achieved if the temperature oscillates from one limit of the temperature interval to another. The values of the parameters of the controller for which this condition is met are then taken to be optimal.

The region of fast motion of the cooler. The results of experiments and simulation calculations confirmed that the control of the temperature in an open-loop unstable state is reliable and simple if the cooler has a fast response. The rate of response of cooler may be characterized by a time t_c during which the cooler traverses from one extreme position to another. If the traverse time of the cooler is less than 398·5 s, it is necessary to use the relay with hysteresis algorithm instead of the ideal relay one, in order to avoid oscillation of the relay due to the noise. This means that the control action must be delayed in order to keep the temperature in the requested interval. Examples of measured results are shown in Figs 1 and 2. The dependence of the temperature overshoot on the rate of traverse of the cooler is shown in Fig. 3. For the traverse time less than 102 seconds the action is fast enough to permit the choice of the switching difference T_{reg} practically equal the requisted tolerance of the temperature ΔT_{reg}. For lower response of the cooler one has to diminish the switching difference in order to compensate for the inertia of the cooler. The limiting situation which restricts the use of the realy with hysteresis algorithm is the case when the switching difference T_{reg} equals the choice band in the temperature ΔT_n. Thus the

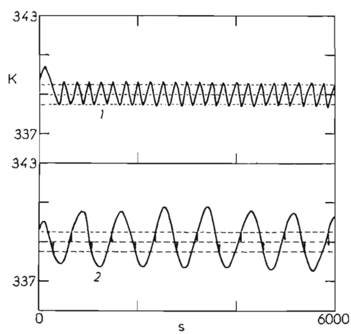

FIG. 1

Examples of experimental time dependences of the reaction temperature for the relay with hysteresis algorithm for $T_{reg} = 0·5$ K, $\Delta T_{reg} = 0·5$ K, $\Delta T_n = 0·01$ K, $T_s = 339$ K. *1* $t_c = 4·8$ s; *2* 234·5 s. The arrows show instant of switching the cooling (↓ the cooler submerges, ↑ the cooler is retracted)

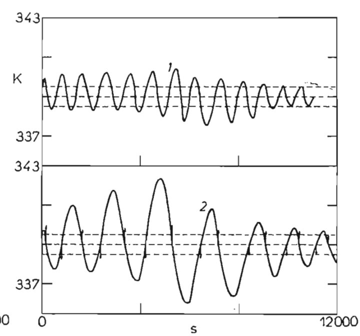

FIG. 2

Examples of experimental time dependences of the reaction temperature for the ideal relay algorithm for conditions as in Fig. 1. *1* $t_c = 398·5$ s; *2* 811 s relay with hysteresis altorithm changes to the ideal relay one, which in the absence of noise would switch exactly upon reaching the requested temperature. In real situations one has to respect the noise and keep a certain switching difference. within the noise band the controller preserves the prevailing status.

Under the control in an unstable point the loop with the ideal relay or the relay with hysteresis algorithms is unstable. This mean that the cooler must reach one or both extreme positions (fully submerged or fully retracted cooler). If the cooler hits only one extreme position, it will be the one that is closer to the extent of submersion corresponding to a pseudostationary state of the reactor. With high requirements on the utilization of the cooling surface the cooler reaches up to full submersion: with low requirements up to full retraction. The magnitude of the overshoot is then determined by the smaller distance from the extreme position. The overshoot is thus maximal if the pseudostationary state corcesponds to half-submerged cooler.

The region of slow motion of the cooler. For the time of traverse of the cooler greater than 811 seconds the ideal relay algorithm does not ensure maining of the temperature within the prescribed interval. Neither does it ensure safe operation and the temperature increases uncontrolably, *i.e.* we have a typical runaway. From this limit we must apply the PD regulator which switches with phase lead.

A fundamental problem encountered with slow coolers is the reactor start-up. In the studied case the reactor was started with fully submerged cooler. The reaction temperature decreased. Upon reaching the requested temperature T_s the catalyst was injected and the cooler was initiated to move upwards. This ensured that the experiments were carried out under the conditions when the reactor had a sufficient cooling capacity to remove the reaction heat. The first switching point thus does not

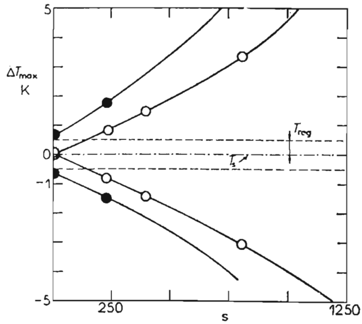

FIG. 3

The effect of the traverse time of the cooler t_c on reaction temperature overshoot. Empty circles designate the ideal relay, full circles the relay with hysteresis control algorithm

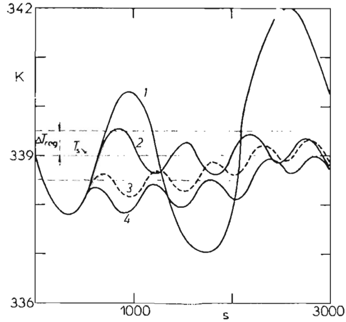

FIG. 4

The effect of the derivative element gain in the PD controller on the course of the reaction temperature for conditions as in Fig. 1 and for $t_c = 811$ s. Results of simulation calculations. *1* $D_k = 50$ s, *2* 100 s, *3* 300 s, *4* 600 s

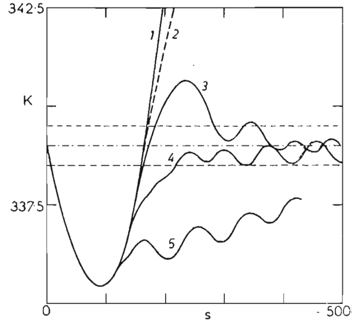

FIG. 5

The effect of the derivative element in the PD controller on the course of the reaction temperature for conditions as in Fig. 1 and $t_c = 1\,684$ s. Results of simulation calculations. *1* $D_k = 0$ s, *2* 250 s, *3* 300 s, *4* 600 s, *5* 1 800 s

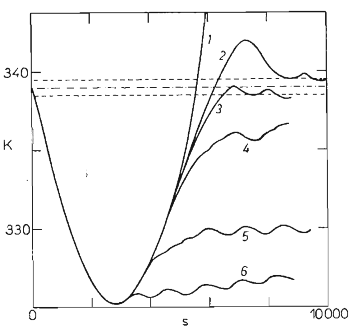

FIG. 6

The effect of the derivative element gain in the PD controller on the course of the reaction temperature for conditions as in Fig. 1 and $t_c = 3\,505$ s. Results of simulation calculations. *1* $D_k = 1\,700$ s *2* 1 750 s, I 800 s, fi 3 000 s, *5* 10 000 s, *6* 30 000 s

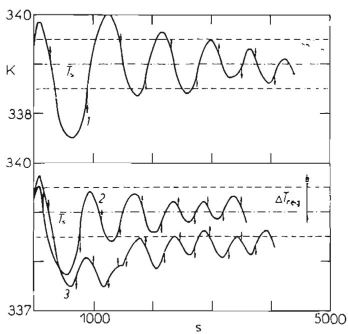

FIG. 7

Experimentally determined effect of the derivative element gain of the PD controller on the course of the reaction temperature for $t_c = 811$ s and other conditions as in Fig. 1, *1* $D_k = 75$ s, *2* 100 s, *3* 600 s satisfy the condition for switching by the PD regulator. Instead, it corresponds to switching by the ideal relay algorithm. This introduces overregulation (subcooling of the reaction mixture) into the start-up period of the process and the regulator then must cope with the start-up of a subcooled reaction mixture. This situation

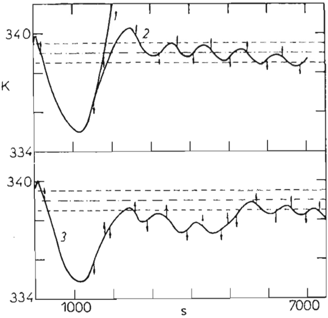

FIG. 8

Experimentally determined effect of the derivative element gain of the PD controller on the course of the reaction temperature for $t_c = 1\,684$ s and other conditions as in Fig. 1, *1* $D_k = 0$ s, *2* 300 s, *3* 600 s

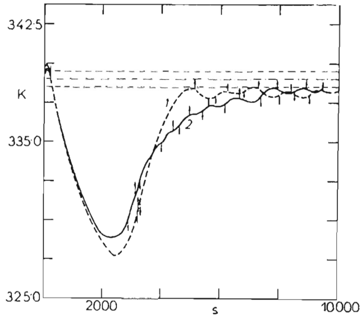

FIG. 9

Experimentally determined effect of the derivative element gain of the PD controller on the course of the reaction temperature for $t_c = 3\,503$ s and other conditions as in Fig. 1, *1* $D_k = 1\,700$ s, *2* 1 800 s

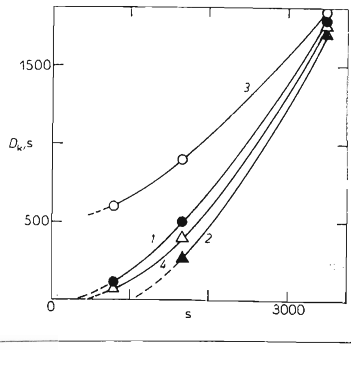

FIG. 10

The range of the derivative element gain of the PD controller as a function of the traverse time of the cooler t_c. *1* Optimum D_k. 2 maximum gain above which an uncontrolable temperature runaway occurs, *3* minimum gain for adequate course of the reaction temperature, *4* minimum gain for which "floating" course of the reaction temperature is observed resembles the start-up of an industrial reactor, where the reaction mixture is gradually heated and the control commences by switching from the cooling to the heating mode. The results of the simulation calculations (Figs 4–6) and the experimental results (Figs 7–9) thus also demonstrate the capability of the PD regulator to cope with the transition from the heating to the cooling mode. The gain of the derivative element of the controller thus changes the temperature which initiates the cooling of the reactor, *i.e.* the temperature which triggers submersion of the cooler. For fast coolers the start-up posed no problem; for slow coolers the start-up was extraordinarily sensitive to the moment of commencing the control.

The limits of applicable gain. The minimum gain of the derivative element of the PD regulator which may be used is determined by stability of the control loop. Since the critical conditions for the control occur at the start-up, this minimum value is set by the value for which the start-up is still feasible.

Increased requirements at the beginning occur due to the fact that the first switching does not obey the rules of the PD controller. The maximum applicable gain is limited by two consequences of the amplification. High gain on the one hand leads to switching prior to reaching the prescribed temperature. This is, as a rule, undesirable as it prolongs the time necessary to reach the prescribed temperature. The other limitation is the amplification of the effect of noise which may cause that the controller does not maintain the temperature at the prescribed level, but off the requiested interval. Under slow motion of the cooler the two effects act in opposite. From the standpoint of ensuring stability one needs maximum possible gain while from the standpoint of reducing the noise, small gain. The interval within which one can ensure a satisfactory and safe control is then narrow leaving only a small margin for practical realization. The range of gain of the derivative element of the PD regulator for moderate and slow motion of the cooler is shown in Fig. 10.

CONCLUSION

The results of this study suggest that the range of speeds of motion of the cooler, within which one can reliably realize the temperature control by the above PD regulator, is not much wider than the interval of applicability of much simpler control algorithms. This result thus shows that it is much more efficient to contain the problems of the control by proper reactor design offering fast response action variables, than to correct ill design and unsuitable action variables by complicated control algorithms.

LIST OF SYMBOLS

A_n value of manipulated variable corresponding to given noise (K)
A_v manipulated variable (Eq. (*6*)) (K)
c_{A0} initial concentration of hydrogen peroxide (kmol m^{-3})

D_k	gain of the derivative element of the PD regulator (s)
$f(x)$	functional dependence of reaction rate on conversion
k	constant in Eq. (*1*)
r	reaction rate (kmol m^{-3} s^{-1})
R	gas constant
t	reaction time (s)
t_c	time of traverse of cooler between extreme positions (s)
T	temperature of reaction mixture (K)
T_s	requested temperature of the reaction mixture (K)
T_{reg}	hysteresis of the controller (K)
x	degree of conversion of hydrogen peroxide
Δt	time to change the reaction temperature by ΔT_s (s)
ΔT_n	band noise in temperature (K)
ΔT_{reg}	requested tolerance for temperature control (K)
ΔT_s	given temperature interval for evaluation of the derivative of temperature with respect to time (K)

REFERENCES

1. Horák J., Jiráček F.: Chem. Eng. Sci. *35*, 485 (1980).
2. Horák J.: 7-th CHISA Congress, Prague 1981.
3. Hengstenberg J., Sturm B., Winkler O.: *Messen, Steuern und Regeln in der Chemischen Technik*, Band III. Springer, Berlin (1981).
4. Amundson N. R., Aris R.: Chem. Eng. Sci. *7*, 121 (1958); *11*, 199 (1959).
5. Gilles E. D.: Chem.-Ing.-Tech. *40*, 469 (1968).
6. Dubil H., Gaube J.: Chem.-Ing.-Tech. *45*, 529 (1973).
7. Horák J., Jiráček F., Ježová L.: This Journal *47*, 446 (1982).
8. Horák J., Jiráček F., Ježová L.: This Journal *47*, 251 (1982).
9. Jiráček F., Horák J.: This Journal *48*, 449 (1983).

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