TEMPERATURE CONTROL IN A CHEMICAL REACTOR THROUGH VARIABLE AREA OF THE HEAT TRANSFER SURFACE. SIMULATION ANALYSIS

Josef HORÁK and Zina VALÁŠKOVÁ

Department of Organic Technology,
Prague Institute of Chemical Technology, 166 28 Prague 6

Received June 10th, 1980

An algorithm has been developed and on a mathematical model analyzed to stabilize the reaction temperature of a batch reactor: The reaction has been a zero-order one and the reactor has been operated in an instable operating point. The action variable is the heat exchange surface whose area is increased if the temperature is above, or decreased if the temperature is below the set point. The following two-point regulators have been studied: An ideal relay, a relay with hysteresis and an asymmetric PD relay. The effect has been discussed of the parameters of the regulators on the quality of regulation. Stability analysis has been made of the stationary switching cycles and the domains of applicability have been determined for individual regulators with respect to the rate of change of the area of heat exchange surface.

The results of our previous studies have lead us to the conclusion that the system dynamic properties are of fundamental importance for the reactor temperature control in an open-loop instable operating point. If the effect of the system time lag is small the temperature of the reactor can be maintained in the instable operating point safely and easily with the aid, of a simple regulator such as for instance, the relay with hysteresis[1-3]. On the contrary, if the system lags heavily the control in an instable operating point is impossible even with the aid of complex control algorithms.

In temperature control through the flow rate of the coolant, or through the temperature of the coolant a very serious problem poses the inertia of the cooling system[4-7]. If the wall of the reactor is thick, or if the hold-up of the coolant in the jacket is large, the control through the inlet temperature of the coolant causes difficulties brought about by the large thermal capacity of the cooling system. A way of avoiding the adverse effect of the inertia of the cooling system is through the use of the area of heat exchange surface as the action variable. The area of heat exchange surface can be varied by a mobile cooling coil immersed to a different depth into the reaction mixture, or by insulating part of the exchange surface.

This paper presents results of a study of the control of a batch reactor by retractable cooling coil. The aim was to delimit the properties of the cooling system required for a succesful control of temperature in an instable operating point with the aid of a two-point regulator.

THEORETICAL

The Mathematical Model of the Reactor

For the calculations we selected a model of the batch reactor based on the following assumptions: perfect mixing of the reaction mixture and the coolant, constant heat transfer coefficient, constant physical properties of the mixture and the coolant, negligible effect of the heat due to the dissipation of the energy supplied by the impeller, negligible heat losses to the surroundings. A zero-order reaction, *i.e.* negligible effect of the degree of conversion on the reaction rate within a single switching cycle was considered.

A balance of heat in the reaction mixture then reads

$$\frac{\mathrm{d}T}{\mathrm{d}t} = (r/c_{\mathrm{A0}})\, T_{\mathrm{ad}} - (k_{\mathrm{h}}A/Vc_{\mathrm{p}}\varrho)\,(T - T_{\mathrm{c}})\,. \qquad (1)$$

Since the aim of this work was a study of the temperature control of the reaction mixture by a coolant with a large thermal capacity (*i.e.* the time constant of the cooler is much larger compared to the time constant of immersion) but small reserve in the cooling capacity (*i.e.* the temperature of the cooler is close to the inlet temperature of the coolant), it was permissible to assume that the temperature of the cooler remained constant within a switching cycle and equaled the inlet temperature of the coolant. Further it was assumed that the cooler moves at the same speed during immersion and retraction and that the area of heat transfer surface varies linearly with time. The speed of this motion is constant and cannot be varied

$$\frac{\mathrm{d}A}{\mathrm{d}t} = (\pm)\,\frac{A_{\mathrm{s}}}{t_{\mathrm{s}}}\,; \quad A \in \langle 0; A_{\mathrm{m}}\rangle\,. \qquad (2)$$

For the description of the reaction rate we have adopted the following zero-order reaction rate equation

$$(r/r_{\mathrm{s}}) = \exp\left[(T - T_{\mathrm{s}})\, E/RTT_{\mathrm{s}}\right]. \qquad (3)$$

The choice of the dimensionless time is based on this concept: Let us assume that the temperature is to be kept at a set point T_{s} with a tolerance $\pm 0{\cdot}5T_{\mathrm{reg}}$. For the characteristic time constant of the regulation process we took the time during which the temperature of the reaction mixture under ideal adiabatic conditions changes from a value $(T_{\mathrm{s}} - 0{\cdot}5T_{\mathrm{reg}})$ to $(T_{\mathrm{s}} + 0{\cdot}5T_{\mathrm{reg}})$ at the reaction rate corresponding to the required temperature. Then we may write

$$t_{\mathrm{reg}} = T_{\mathrm{reg}}c_{\mathrm{A0}}/T_{\mathrm{ad}}r_{\mathrm{s}}\,. \qquad (4)$$

For the dimensionless time we took the ratio of the real time to the characteristic time constant of the regulation process

$$\tau = t/t_{\mathrm{reg}}\,. \tag{5}$$

The dimensionless temperature was taken as a deviation of the instantaneous temperature from the ideal steady state value scaled by the adiabatic temperature rise

$$\theta = (T - T_s)/T_{\mathrm{ad}}\,; \quad \theta_c = (T_c - T_{cs})/T_{\mathrm{ad}} \tag{6}$$

The dimensionless area of the heat exchange surface was taken as the instantaneous heat exchange surface devided by the value of the corresponding steady state

$$P = A/A_s\,. \tag{7}$$

After rendering dimensionless, Eqs (*1*) and (*2*) take the following form

$$\frac{\mathrm{d}\theta}{\mathrm{d}\tau} = \frac{T_{\mathrm{reg}}}{T_{\mathrm{ad}}}\left\{\frac{r}{r_s} - P\left[1 + \frac{T_{\mathrm{ad}}}{T_s - T_{cs}}(\theta - \theta_c)\right]\right\} \tag{8}$$

$$\frac{\mathrm{d}P}{\mathrm{d}\tau} = \pm\,\frac{T_{\mathrm{reg}}c_{A0}}{T_{\mathrm{ad}}r_s t_s}\,. \tag{9}$$

Linearization of Equations

For the description of the behaviour in the vicinity of the steady state we have adopted the following simplifying assumptions:

The reaction rate is a linear function of temperature:

$$r/r_s = 1 + B\theta\,, \tag{10}$$

where $B = ET_{\mathrm{ad}}/RT_s^2$.

Since the temperature of the reaction mixture varies only little compared to the area of heat transfer surface we may assume that

$$P(\theta - \theta_c) = P(\theta_s - \theta_{cs}) = 0\,. \tag{11}$$

Eqs (*8*) and (*9*) then change into the following form

$$\frac{\mathrm{d}\theta}{\mathrm{d}\tau} = D(1 + B\theta - P) \tag{12}$$

$$\frac{dP}{d\tau} = \pm M . \tag{13}$$

The Control Algorithms

Three algorithms have been tested. For all three cases it has been assumed that the regulator has two positions: in one position the cooler is being immersed or has been entirely submerged ($A = A_m$); in the other position the cooler is just emerging or has been entirely retracted ($A = 0$). For the fast motion of the cooler we have used the algorithm "relay with hysteresis"; the hysteresis prevents rapid oscillations of the relay in the neighbourhood of the operating point. For the slower motion of the cooler we have utilized the "ideal relay" algorithm. For the temperature control with the slow motion of the cooler one can use the asymmetric PD algorithm, ment to prevent primarily the undesirable temperature rise. A review of the conditions of switching is given in Table I.

Solution of the Mathematical Model

Two limiting cases may occur during the switching cycle:

1) The cooler moves from one extreme position ($P = 0$) into the other ($P = P_m$). The course of the switching cycle is unambiguously determined by the temperature of the reaction mixture, θ_n, at the beginning of the switching cycles and the switching cycles are independent to each other. The limit switching cycles may therefore be found as a solution of Eqs (*12*), (*13*) with the initial conditions corresponding to individual studied algorithms.

The switching cycle proceeds in four steps: *a*) Immersion of the cooler – the area of the heat transfer surface changes from $P_n = 0$ to $P_1 = P_m$. *b*) Cooling – the area

TABLE I

A review of switching conditions for used algorithms

Algorithm No	Name	Condition determining the state when the cooler is being immersed or has been fully immersed
I	ideal relay	$T > T_s$
II	relay with hysteresis	$(T > T_s + 0{\cdot}5h) \vee [(dT/dt < 0) \wedge$ $\wedge\ (T > T_s - 0{\cdot}5h)]$
III	asymmetric PD regulator	$(T > T_s) \vee [(T < T_s) \wedge$ $\wedge\ (T - T_s + a(dT/dt)) > 0]$

of heat transfer surface is at its maximum ($P = P_m$). *c*) Retraction of the cooler – the area of heat transfer surface changes from $P_1 = P_m$ to $P_{n+1} = 0$. *d*) Adiabatic heating of the reaction mixture – the area of heat transfer surface is zero, the reaction mixture is heated by the reaction heat.

2) The cooler does not move as far as the extreme position and the course of the switching cycle depends both on the initial temperature of the reaction mixture, θ_n, as well as on the initial value of the area of heat transfer surface, P_n. The switching cycle goes through steps *a*) and *c*), while we have that $P_n > 0$ and $P_1 < P_m$.

TABLE II

The initial conditions

General designation of the initial conditions

Step of the switching cycle	time τ	cooling surface P	temperature of the mixture θ
a)	$\tau_p = 0$	P_n	θ_n
	τ_1	P_1	θ_1
b)	τ_1	P_1	θ_1
	τ_k	P_1	θ_k
c)	τ_p	P_1	θ_k
	τ_2	P_{n+1}	θ_2
d)	τ_2	P_{n+1}	θ_2
	τ_{k2}	P_{n+1}	θ_{n+1}

Concrete values of initial conditions for individual algorithms

1 — Surface area $P \in \langle 0; P_m \rangle$

Algorithms	θ_2	τ_p	P_n	θ_n	τ_1	P_1	θ_1	θ_k	τ_2	P_{n+1}	θ_{n+1}
I	θ_2	0	0	0	τ_c	P_m	θ_1	0	τ_c	0	0
II	θ_2	0	0	$H/2$	τ_c	P_m	θ_1	$-H/2$	τ_c	0	$H/2$
III	θ_2	0	0	θ_{n-1}[a]	τ_c	P_m	θ_1	0	τ_c	0	θ_{n+1}[a]

2 — Surface area $P \in (0; P_m)$

Algorithms	τ_p	P_n	θ_n	τ_1	P_1	$\theta_1 = \theta_k$	τ_2	P_{n+1}	$\theta_2 = \theta_{n+1}$
I	0	P_n	0	τ_1	$P_1 < P_m$	0	τ_2	$P_{n+1} > 0$	0
II	0	P_n	$H/2$	τ_1	$P_1 < P_m$	$-$ H/2	τ_2	$P_{n+1} > 0$	$H/2$
III	0	P_n	θ_{n-1}[a]	τ_1	$P_1 < P_m$	0	τ_2	$P_{n+1} > 0$	θ_{n+1}[a]

[a] It must hold that ($\theta_n + b \cdot [d\theta/d\tau]_n = 0$).

Initial conditions for individual algorithms and steps of the switching cycle are shown in Table II.

TABLE III

Temperature of the reaction mixture and the area of heat exchange surface as functions of time for individual steps of the switching cycle

Function	Step of the switching cycle			
	a	*b*	*c*	*d*
Temperature	$\theta_a(\tau)$	$\theta_b(\tau)$	$\theta_c(\tau)$	$\theta_d(\tau)$
Area	$P = P_m + M \cdot \tau$	$P = P_m$	$P = P_1 - M \cdot \tau$	$P = 0$
Phase plane	$\theta_a(P)$	—	$\theta_c(P)$	—
Derivative with respect to time	$\frac{d\theta_a(\tau)}{d\tau}$	—	$\frac{d\theta_c(\tau)}{d\tau}$	—

The form of individual functions:

$$\theta_a(\tau) = \frac{P_n - 1}{B} + \frac{M\tau}{B} + \frac{M}{B^2D} + \left(\theta_n - \frac{P_n - 1}{B} - \frac{M}{B^2D}\right) . \exp(BD\tau) \tag{III-1}$$

$$\theta_b(\tau) = \left(\theta_1 - \frac{P_m - 1}{B}\right) . \exp[BD(\tau - \tau_1)] + \frac{P_m - 1}{B} \tag{III-2}$$

$$\theta_c(\tau) = \frac{P_1 - 1}{B} - \frac{M\tau}{B} - \frac{M}{B^2D} + \left(\theta_k - \frac{P_1 - 1}{B} + \frac{M}{B^2D}\right) . \exp(BD\tau) \tag{III-3}$$

$$\theta_d(\tau) = \left(\theta_2 + \frac{1}{B}\right) . \exp[BD(\tau - \tau_2)] - \frac{1}{B} \tag{III-4}$$

$$\theta_a(P) = \frac{P - 1}{B} + \frac{M}{B^2D} + \left(\theta_n - \frac{P_n - 1}{B} - \frac{M}{B^2D}\right) . \exp\left[\frac{BD}{M}(P - P_n)\right] \tag{III-5}$$

$$\theta_c(P) = \frac{P - 1}{B} - \frac{M}{B^2D} + \left(\theta_k + \frac{M}{B^2D} - \frac{P_1 - 1}{B}\right) . \exp\left[\frac{BD}{M}(P_1 - P)\right] \tag{III-6}$$

$$\frac{d\theta_a(\tau)}{d\tau} = \frac{M}{B} + BD\left(\theta_n - \frac{P_n - 1}{B} - \frac{M}{B^2D}\right) . \exp(BD\tau) \tag{III-7}$$

$$\frac{d\theta_c(\tau)}{d\tau} = \frac{-M}{B} + BD\left(\theta_k - \frac{P_1 - 1}{B} + \frac{M}{B^2D}\right) . \exp(BD\tau) \tag{III-8}$$

On integrating Eqs (*12*) and (*13*) and on substituting the general initial conditions from Table II, the time dependences of the temperature of the reaction mixture and the area of the heat transfer surface are obtained for individual steps of the switching cycle. Transforming Eqs (*12*) and (*13*) into the $\theta - P$ plane and solving the resulting set, the dependence of the temperature of the reaction mixture was obtained as a function of the area of heat transfer surface during immersion or retraction of the cooling coil. The obtained equations and their derivatives are shown in Table III.

The Domain of Attraction of the Algorithms

By the domain of attraction it is ment the interval of P_n and M values within which, after completion of a switching cycle, the temperature θ_n of switching is reached again.

In the domain of attraction we must have

$$(\mathrm{d}\theta_a/\mathrm{d}\tau = 0 \quad \text{for} \quad P < P_m) \wedge (\mathrm{d}\theta_c/\mathrm{d}\tau = 0 \quad \text{for} \quad P > 0)\,. \qquad (14)$$

This means that the maximum (θ_{amax}) or minimum (θ_{cmin}) temperature must be reached at the time when the area of the heat exchange surface is being changed.

If the temperature maximum is reached at the instant when $P = P_m$, then the speed of motion of the cooler, M, and the area of the cooling surface at the beginning of the switching cycle, P_n, satisfy the following condition

$$0 = P_{nmin} - P_m + \frac{M_{min}}{BD} \ln \{M_{min}/[M_{min} - B^2 D\theta_n + BD(P_{nmin} - 1)]\}\,. \qquad (15)$$

At the same time the surface area in the domain of attraction $P = P_{n+1}$, whose value is determined by Eq. (*III-6*) with the parameters $P_1 = P_m$, $\theta_c = \theta_n$ and $M \equiv M_{min}$, must fulfill the following inequality

$$P_{n+1}((III\text{-}6)) \geqq P_{nmin}((17))\,. \qquad (16)$$

This ensures that while the cooler is retracted (step *c*) the system would not leave the domain of attraction.

The conditions (*16*) and (*15*) determine the limits of the domain of attraction of individual control algorithms. A combination of the constants P_{nmin} and M_{min} delimits minimum possible values; constants above those given by Eq. (*15*) permit use of the given control algorithm, while for lower values of these constants the given algorithm is inaplicable for it causes either the reaction to extinguish or leads to a runaway temperature due to inadequate cooling.

Conditions (*15*) and (*16*) are necessary but not sufficient for the given algorithm to satisfy the requirements put on the temperature control. Further it must hold

$$(0 < \theta_{\mathrm{amax}} \leqq +0{\cdot}5\theta_{\mathrm{reg}}) \wedge (\theta_{\mathrm{cmin}} \geqq -0{\cdot}5\theta_{\mathrm{reg}}) . \qquad (17a,b)$$

This means that a prescribed quality of control must be achieved during the limiting cycle. If the temperature θ is not available with absolute accuracy, *i.e.* there exists a noise band of the width $\pm\varepsilon$, then there is still another inequality that must be fulfilled in order to prevent oscillation of the relay around the steady state due to the random noise

$$(\theta_{\mathrm{amax}} > 2\varepsilon) \wedge (\theta_{\mathrm{cmin}} < -2\varepsilon) . \qquad (18a,b)$$

The mathematical model was solved on a TESLA 200 computer with the following values of the constants: $B = 7{\cdot}809$; $D = 0{\cdot}0125$; $\varepsilon = 3{\cdot}125 \cdot 10^{-4}$; $c_{\mathrm{A0}} = 1\ \mathrm{kmol\ m^{-3}}$; $r_s = 3{\cdot}3 \cdot 10^{-3}\ \mathrm{kmol_A\ m^{-3}\ s^{-1}}$; $E = 90\ \mathrm{kJ\ mol_A^{-1}}$; $T_{\mathrm{ad}} = 80\ \mathrm{K}$; $T_s = 333\ \mathrm{K}$; $T_{\mathrm{reg}} = 1\ \mathrm{K}$; $r_{\mathrm{reg}} = 3{\cdot}79\ \mathrm{s}$.

DISCUSSION

The aim of this work was to study the behaviour of the batch reactor controlled by a mobile cooler, and, in particular, to find out what should be the speed of motion of the cooler in order to obtain a safe control. The speed of motion has been characterized by the dimensionless velocity M. For the analysis we have selected the case of the control in an open-loop instable operating point. The analysis has been focused mainly on the case of a small reserve in the cooling area (about 20%), *i.e.* the area of cooling surface corresponding to the steady state equals 80% of the maximum cooling surface available. The reserve is characterized by the dimensionless parameter P_m (the reserve of cooling of 20% corresponds to $P_m = 1{\cdot}25$).

The Behaviour of the System with the Ideal Relay (algorithm I)

The analysis has shown that the operating point even with the control loop closed remains instable. Examples of the courses of trajectories in the phase plane $\theta - P$ are shown in Fig. 1*a*. If the system is adjusted into the vicinity of the operating point, the deviation of the surface area of the cooler gradually drifts away from the steady state value causing a limiting cycle which is stabilized by fixing the cooler in one of the extreme positions. Which of the extreme positions is reached depends on the reserve of the cooling area. If we have $P_m < 2{\cdot}05$, the limiting cycle is fixed in such a way that a part of the switching cycle experience fully immersed cooler (Fig. 2*a*). On the contrary, if we have $P_m > 2{\cdot}05$, the cooling surface remains zero and the limiting cycle is stabilized in such a way that part of the switching cycle goes adiabatic

(Fig. 2*b*). Examples of the course of limiting cycles for various speeds of motion, M, and constant P_m are shown in Fig. 2.

If the deviations of the temperature during the control by the ideal relay are not to exceed $\pm 0{\cdot}5T_{reg}$, the following conditions must be met: for $P < 2{\cdot}05$ conditions (*17a*), (*18b*) and for $P_m > 2{\cdot}05$ conditions (*17b*) and (*18a*). For the control in the instable operating point the magnitude of the maximum deviation of the temperature from the set point depends on the one hand on the reserve in the cooling area (parameter P_m), and, on the other hand, on the speed of motion of the cooler.

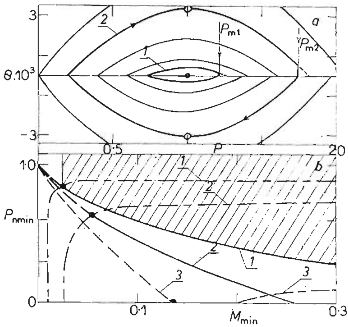

FIG. 1

The ideal relay. *a*) The course of trajectories in the Θ–P plane; $M = 1{\cdot}25$; ● — operating point; ○ — Θ_{amax}, Θ_{cmin}; ——— stable limit cycle; *1* $P_{m1} = 1{\cdot}25$; *2* $P_{m2} = 1{\cdot}75$. *b*) The limits of the domain of attraction; P_m: *1* 1·1; *2* 1·25; *3* 1·75; –·–·– $P_n = f(M_{min})$ — Eq. (*III-6*); ———, ----- $P_{nmin} = f(M_{min})$ — Eq. (*15*); ——— the limits of the domain of attraction; //////// — the domain of attraction for $P_m = 1{\cdot}1$

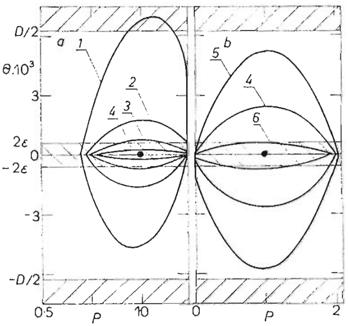

FIG. 2

The ideal relay — the course of limit cycles in the phase plane *a*) $P_m = 1{\cdot}25$; *b*) $P_m = 2{\cdot}5$; ● — operating point; M: *1* 0·1; *2* 0·26; *3* 0·63; *4* 2·5; *5* 1·25; *6* 10·0

The fact that the limiting cycle is stabilized by reaching one of the extreme positions of the cooler causes that the maximum deviation of the temperature at constant speed of motion depends on the reserve of the cooling surface (Fig. 1*a*), *i.e.* on the distance of the steady state position of the cooler from the nearest extreme position. The maximum deviation of the temperature corresponds to the value $P_m = 2 \cdot 05$, *i.e.* to the case when the steady state position of the cooler is half-way between the extreme positions.

The speed of motion of the cooler acts in general in such a way that the deviation of the temperature decreases with increasing speed of motion of the cooler. In the

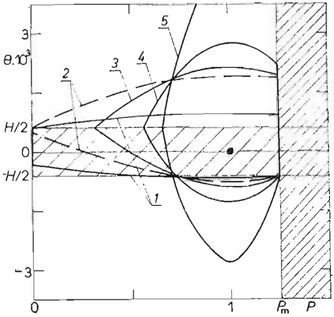

FIG. 3

The relay with hysteresis — the course of limit cycles in the phase plane. $P_m = 1 \cdot 25$; $H = 1 \cdot 25 \cdot 10^{-3}$; M: *1* 20; *2* 5; *3* 2; *4* 0·6; *5* 0·2; //////// — the region of hysteresis; ● — operating point

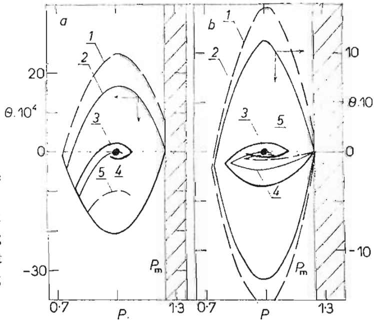

FIG. 4

The asymmetric PD regulator — the course of trajectories in the phase plane. $P_m = 1 \cdot 25$; ● — operating point, *a*) The effect of parameter b: $M = 0 \cdot 2$; b: *1* $1 \cdot 1 \cdot 10^{-2}$; *2* 0·12; *3* 0·43; *4* 0·51; *5* 0·9, *b*) The effect of parameter M: $b = 5 \cdot 10^{-2}$; $M =$ *1* 0·26; *2* 0·31; *3* 1·25; *4* 1·7; *5* 5·0 practical situation one has to seek a compromise. Excessive speeds of motion of the cooler diminish the temperature variations during the switching cycle below the level of the random noise. Examples are shown in Fig. 2*a* – curve *4*, Fig. 2*b* – curve *6*. At the speed of motion $M < 0{\cdot}11$ (for $P_m = 1{\cdot}25$) the temperature deviation exceeds already the level $\pm 0{\cdot}5T_{reg}$ and the control does not meet the requested standard. The range of suitable speeds of motion of the cooler for the control by the ideal relay ($P_m = 1{\cdot}25$) is shown in Fig. 5 – curves *3*. The limits of the domain of attraction for the given algorithm (*i.e.* the range of combinations of the parameters M and P_n for which the control does not fail) for different values of the cooling reserve are shown in Fig. 1*b*.

The Behaviour of the System with the Relay with Hysteresis

Introducing hysteresis into the function of the relay serves as safeguard against the effect of random noise. Hysteresis deteriorates the properties of the regulation process in that the deviations from the set point are increased by hysteresis.

Even for the relay with hysteresis the operating point remains instable. At high speeds of motion of the cooler the limiting cycle is stabilized in that the cooler hits the extreme positions at both ends and the switching cycle takes place partially under the adiabatic condtitions, partially at full intensity of cooling. If the speed of motion of the cooler is extremely high ($M > 20$) the temperature variations during the motion of the cooler are negligible and the temperature remains within the range of hysteresis. An example is shown in Fig. 3 – curve *1*.

At small speeds of motion of the cooler ($M < 5$) the whole area of cooling surface is no longer utilized and the system behaves analogously to that with the ideal relay; maximum temperature deviation increases with decreasing speed of motion of the cooler. The effect of the magnitude of the reserve area of cooling surface is also analogous to the ideal relay case.

The quality of the regulation decreases with the width of hysteresis; examples are shown in Fig. 5 – curves *1*, and *2* which also show the range of suitable speeds of motion of the cooler for the control of the reactor by a relay with hysteresis.

In practical use of the relay with hysteresis one can achieve the purpose of the control only if the band width of hysteresis is smaller than the tolerated deviation of the temperature T_{reg}. This can be met only then if the band width of random noise is much smaller than the tolerated deviation of the temperature.

The Behaviour of the System with the Asymmetric PD Algorithm

An asymmetric algorithm was used in order to suppress primarily the temperature rise, representing in case of the temperature control serious hazard, while the temperature decrease is by far not so dangerous. In examining this algorithm we have another variable, the gain of the derivative component in Eq. (*19*) describing the regulator. After rendering it dimensionless the equation takes the form

$$\frac{\mathrm{d}\theta}{\mathrm{d}\tau} \cdot b + \theta = 0 \,. \tag{19}$$

It has been found out that for the case that the function (*III-3*), describing the course of the temperature of the mixture, is convex during retraction of the cooler, *i.e.* if the following condition is met

$$(1 - P_1) \cdot B \cdot D + M > 0 \tag{20}$$

there exists always such a derivative constant, b, ensuring stability of the operating point. This signifies that the operating point may be stable and the control leads to formation of an infinitesimally close limit cycle around the operating point (in practice the limit cycle is not infinitely close but its distance from the operating point is given by the lags, delays and other non-idealities of the control loop).

The effect of the speed of motion of the cooler, M, and of the dimensionless derivative constant, b, on the course of the switching cycles is similar. According to the values of the parameters the following situations may occur:

1) Too small a value, *i.e.* small speed of motion of the cooler or a small derivative constant. The operating point is instable; there exists a stable limit cycle stabilized by reaching the extreme position of the cooler (P_m). The behaviour is analogous to the case of relay. Examples are shown in Fig. 4*a*,*b* – curves *1*. If the temperature of switching, θ_s, is reached at the instant when $P = P_m$, then the given parameters M or b are at the low limit of the stability region (Fig. 4*a*,*b* – curves *2*).

2) The operating point is stable. This means that the deviation of the surface area of the cooler, as well as the deviation of the temperature from the steady state value, diminish and form a limit cycle inifinitely close to the operating point. An example is shown in Fig. 4*a*,*b* – curve *3*. If the maximum temperature reached during the switching cycle just equals the requested value, θ_s, the given parameter is just at the upper limit of the stability region.

3) Too high a value of the parameter (Fig. 4*a*,*b* – curves *5*). The operating point is instable and there exists no limit cycle in its near vicinity. During retraction of the cooler the requested temperature of the set point, θ_s, is not reached and, unless the cooling is terminated, the reaction extinguishes. This parameter region is not very suitable for control purposes.

Examples of the course of the switching cycles in dependence on the magnitude of the parameters are shown in Fig. 4*a* – the effect of the derivative constant b, in Fig. 4*b* – the effect of the speed of motion of the cooler M. The extent of the stability region is shown in Fig. 5 – curves *4*.

The Region of Applicability of Individual Algorithms

The most important factor affecting the selection of the algorithm is the speed of motion of the cooler and the band width of the random noise. The region of applicability of individual algorithms in dependence on the speed M is shown in Fig. 6.

At high speed of motion of the cooler it is necessary to use a relay with hysteresis. For the speed M exceeding 20, the temperature of the reaction mixture practically does not exceed the region of hysteresis; for M between 0·21 and 20 the temperature remains within the tolerance of θ_{reg}. The relay with hysteresis thus enables a reliable control of the temperature for the speeds of the cooler $M > 0{\cdot}21$.

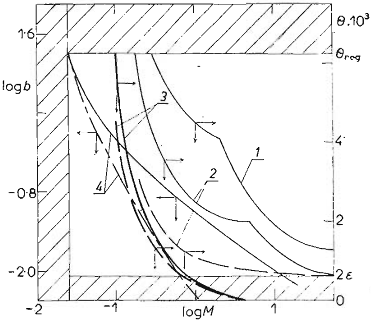

FIG. 5

Region of applicability of individual algorithms – the dependence of the quality of regulation, or the derivative constant b on the speed of motion of the cooler. $P_m = 1{\cdot}25$; ——— Θ_{amax}; ----- Θ_{cmin}. Relay with hysteresis: *1* $H = 8\varepsilon$; *2* $H = 4\varepsilon$. The ideal relay: *3*; The asymmetric PD regulator: *4* ——— b_{max}; ////// b_{min}

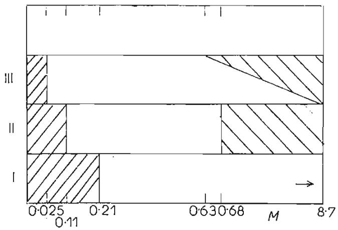

FIG. 6

Scheme of applicability of individual algorithm (*I*–*III*) in dependence on the speed of motion of the cooler M $P_m = 1{\cdot}25$; //////// – Θ_{reg} exceeded; \\\\\\ – lost in noise. Algorithms are to be marked by Roman numerals in sequence *III*, *I*, *II* from the top

For smaller speed of motion of the cooler, $0.11 < M < 0.68$, the deviations from the set point begin to assume appreciable values and it is necessary to change to a more perfect algorithm – the ideal relay. Since the inertia of the system causes a relatively slow drift of temperature around the set point, T_s, the danger of oscillations in the neighbourhood of the operating point appears to be small.

For very small speed of motion of the cooler ($M < 0.11$) it is necessary to use a more complex algorithm, *i.e.* the PD control. With the decreasing speed of motion of the cooler, the conditions for the control become more exacting and the safety margin of the operation decreases as well. This becomes manifest in two ways: On the one hand the interval of values of the gain of the regulator leading to stable operating point grows narrower (Fig. 5 – curves *4*). On the other hand, the domain of attraction of the operating point also narrows. This gives rise to difficulties, especially during the start-up as it can no longer be realized by applying the given algorithm to the state of fully retracted cooler. Such a procedure would lead to an uncontrolled temperature runaway even before the cooler could be sufficiently immersed to offset the temperature growth. The narrowing of the interval of values of b becomes more exacting as far as the accuracy of setting the regulator is concerned and increases the parametric sensitivity of the system.

From the analysis it follows that for low speeds of motion of the cooler there is not much chance that this deficiency could be countered by a more sophisticated algorithm. This also suggests that a proper way to a safe operation is primarily a sufficient speed of the cooler. The question of proper algorithm is only secondary.

CONCLUSION

The results of the mathematical analysis indicate that a mobile cooler offers an effective way of temperature control in chemical reactors even in the instable operating point.

The advantages of the proposed method of control are following: The dynamic properties of the action variable can be chosen independently of the remaining properties of the system and the reaction by selecting a proper speed of motion for the cooler.

It is possible to apply high flow rates of the coolant and hereby achieve a fast response of the cooler and small temperature variations of the coolant. This decreases sensitivity of the coolant to the change in the progress of the reaction (reactivity *etc.*) and the behaviour of the system simplifies.

Large thermal capacity may serve for controlling the fast evolution of heat at the onset of the reaction.

The above advantages could outweigh the increased costs of the reactor and more complicated construction.

LIST OF SYMBOLS

A	area of heat exchange surface (m^2)
A_m	maximum area of heat exchange surface (m^2)
$a > 0$	derivative constant (s)
B	dimensionless constant in Eq. (*10*)
$b = a/t_{reg}$	dimensionless derivative constant
c	concentration ($kmol\ m^{-3}$)
c_p	specific heat ($J\ kg^{-1}\ K^{-1}$)
$D = T_{reg}/T_{ad}$	dimensionless band width of regulator
E	activation energy ($J\ mol_A^{-1}$)
$H = h/T_{ad}$	dimensionless band width of hysteresis
h	band width of hysteresis (K)
k_h	heat transfer coefficient ($J\ m^{-2}\ K^{-1}\ s^{-1}$)
$M = t_{reg}/t_s$	dimensionless speed of motion of the cooler
P	dimensionless area of heat exchange surface
P_m	maximum dimensionless area of heat exchange surface
R	gas constant ($J\ mol^{-1}\ K^{-1}$)
r	reaction rate ($kmol_A\ m^{-3}\ s^{-1}$)
T	temperature (K)
T_{ad}	adiabatic temperature rise (K)
T_{reg}	width of regulation band (K)
t	time (s)
t_s	time to immerse the heat transfer surface A_s corresponding to the steady state (s)
t_{reg}	time constant of the regulation process, Eq. (*4*) (s)
V	volume (m^3)
ε	dimensionless random noise band width
Θ	dimensionless temperature
ϱ	density ($kg\ m^{-3}$)
τ	dimensionless time
τ_c	dimensionless time to fully immerse the cooling surface P_m

Subscripts

A	key component
a, b, c, d	steps a)—d) of the switching cycle
amax	maximum value within a limit cycle
c	coolant
c min	minimum value within a limit cycle
min	minimum
max	maximum
n, n + 1	value at the beginning of the n-th and the (n + 1)-th switching cycle
o	initial value
s	steady state
1, k, 2	values at the end of step a), b) and c) of the switching cycle

REFERENCES

1. Jiráček F., Horák J., Havlíček J.: Chem. Prům. *29*, 4, 209 (1979).
2. Horák J., Sojková Z., Jiráček F., Špačková A.: Chem. Prům. *29*, 9, 456 (1979).

3. Horák J., Valášková Z.: Chem. Prům. *30*, 10, 518 (1980).
4. Luyben W. L., Melcic M.: Hydrocarbon Process *57*, 115 (1978).
5. Marroquin G., Luyben W. L.: Chem. Eng. Sci. *28*, 993 (1973).
6. Hopkins B., Aldorf G. H.: Instr. Tech. *20*, 5, 39 (1973).
7. Oh Se H., Luus R.: AIChE J. *22*, 1, 140 (1976).

Translated by V. Staněk.