A SIMPLIFIED METHOD
OF TEMPERATURE CONTROL MAXIMIZING PRODUCTIVITY
OF THE BATCH REACTOR; THE EFFECT OF INERTIA
OF THE COOLING SYSTEM

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The effect has been studied of the inertia of the cooling system on the reliability of control of the temperature of the reaction mixture. The study has been made using a mathematical model of the batch reactor with an exothermic reaction. The temperature has been controlled by a two--level controller opening and closing the flow of the coolant. The aim of the control has been to maintain a constant value of the degree of utilization of the cooling capacity of the reactor. The instantaneous value of the degree of utilization has been assessed from the ratio of times for which the cooling system is idle to the time of operation. The reliability of control has been studied for variable activity of the catalyst.

A simple method of adaptive control of temperature of the reaction mixture using a mathematical model has been described and experimentally tested in the previous communication[1]. The method utilized a simple two-level controller. The essence of the control method was the evaluation of the degree of utilization of the cooling capacity of the reactor from the time for which the cooling system is idle and the time for which the cooling system is operational. It has been proven that this simplified method permits the temperature of the reaction mixture to be controlled in such a manner as to maintain a constant value of the degree of utilization of the cooling capacity of the system on a present value. An improvement offered by this method of control is a significant increase of reactor's productivity in comparison to the iso-thermal control. These results have been verified on a reactor with a fast response to the effected control action. In such a reactor the actuation of the cooling system becomes manifest through immediate change of the reaction temperature. In real reactors, however, the response of the controlled system need not be very rapid[2-8]. The aim of this work has been to study on a mathematical model the reliability of the method in those cases exhibiting a significant inertia of the cooling system.

THEORETICAL

The mathematical model. The mathematical model is based on the idea of a perfectly mixed batch reactor with an exothermic first-order reaction. The cooling system of the reactor is described by a first-order time-delay element. It is assumed that the concept of a perfectly mixed cooling system may be used with a constant value of the coefficient of heat transfer independent of the flow rate of the coolant. This idea is justified in reactors with recycled coolant. The model operates in the real time in order to facilitate comparison of results with experiments on a laboratory scale set-up. In more detail the mathematical model has been described in the previous communication[1].

The principle of the temperature control. Let us define the real degree of utilization of the cooling capacity of the reactor, R_s, (termed as the degree of utilization, R_s, in the following text), as the ratio of the rate of heat production by chemical reaction to the maximum cooling capacity attainable for the given temperature of the reaction mixture, *i.e.* for the maximum flow rate of the coolant. The aim of the control is to maintain this quantity constant at a present level. In the course of the control the instantaneous value of the degree of utilization of the cooling capacity of the reactor is determined from the response of the temperature of the reaction mixture on the turn-off and the turn-on of the cooling system. This value shall be termed the experimental degree of utilization, R_e, and it is assessed by the following procedure.

After starting the process the temperature of the reaction mixture is $T_{s,1}$, which may be safety assumed to have a corresponding degree of utilization, R_e, less that the present value. The cooling system is turned off, the temperature of the reaction mixture increases by the reaction heat. Having reached the temperature $T_{s,1} + T_{reg}$ the cooling system is actuated and remains active untill the temperature has dropped to $T_{s,1} - T_{reg}$ (the algorithm "relay with hysteresis"). The value of the degree of utilization, R_e is determined from the time t_a, for which the cooling system was idle and the time t_c, for which the cooling system was operational.

$$R_e = t_c/(t_a + t_c) . \tag{1}$$

The temperature interval of the width of the hysteresis band of the controller T_{reg} is taken so as to exceed the band width of random noise.

The value of the degree of utilization then serves to calculate by extrapolation a next value, $T_{s,2}$, for which the degree of utilization just attains the present value and the routine is repeated. By successive repetition of the experimental determination of the degree of utilization and by successive choice of the temperatures $T_{s,n}$ the degree of utilization, R_e, is maintained on the requested constant value. The method of extrapolation of $T_{s,n}$ has been dealt with in detail in the previous communication.

RESULTS AND DISCUSSION

The Quantities Affecting the Rate of Response of the System

With a two-level control the rate of response of the system depends on two quantities. On the ratio of thermal capacities of the reaction mixture and the thermal capacity of the cooling system

$$B = Vc_p\varrho/(V_c c_{pc}\varrho_c) . \qquad (2)$$

The value of the ratio of thermal capacities is fixed by reactor's design, *i.e.* by the volume of the coolant and thermal capacities of the walls of the cooling system. The second parameter is the residence time of the coolant in the cooling system. Its reciprocal is designated as

$$C = F_c/V_c . \qquad (3)$$

The residence time depends on the flow rate of the coolant and for the two-level control takes on either zero or maximum value. For the two-level control the response of the cooling system is asymmetric, for the flow rate of the coolant affects only the rate of the response following the actuation of the cooling system. The higher the selected flow rate of the coolant, the faster the response of the cooling system and the faster the temperature drop within the cooling system. The least value that can be plausibly attained, following the control action then follows from the thermal balance within the cooling system

$$(r/c_{A0}) \Delta T_{ad} = (C/B) (T_c - T_{ci}) \qquad (4)$$

The temperature of the coolant in the cooling system thus depends on the ratio of the parameters B and C.

The rate of response after idling the cooling system cannot be affected for a given design of the reactor, for the rate at which the coolant is heated is determined only by the heat exchange between the content of the cooling system and the reaction mixture. This asymmetric feature need not be harmful from the standpoint of the safety of reactor operation for the fast response can be achieved in the direction which is of prime importance for the safety. Fast cooling of the system therefore ensures also fast quenching of the reaction mixture. This, however, causes also accumulation of "cold" in the cooling system which in turn slows down the rate of temperature increase following the idling of the cooling system.

The Consequences of the Inertia of the Cooling System for Temperature Control

The increased risk of runaway temperature. One of the principal problems of the adaptive control of the batch reactors with batch-to-batch variable properties of the

reaction mixture (reactivity, catalytic activity, activity of the initiator) is the choice of the temperature actuating the cooling system. For the proposed method of control the information about the state of the system from this moment is no longer available. The large inertia of the cooling system causes that the cooling effect lags. Prior to the first actuation of the cooling system the system is heated to the reaction temperature and thus accumulates no "cold". This causes that with increasing inertia of the cooling system the value of the degree of utilization, R_e, at which the control scheme fails already after the first cooling stage (the runaway temperature occurs) grows smaller. Examples of the effect of the thermal capacity of the cooling system (para-

FIG. 1

Start-up of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effects of thermal capacity of the cooling system (parameter B) and the inertia of the temperature sensing device: $A = 0.001\ s^{-1}$, $\Delta T_{ad} = 130\ K$; $1\ B = 50$, $C = 0.7\ s^{-1}$, $\tau_t = 1\ s$; $2\ B = 10$, $C = 0.14\ s^{-1}$, $\tau_t = 1\ s$; $3\ B = 5$, $C = 0.07\ s^{-1}$, $\tau_t = 1\ s$; $4\ B = 50$, $C = 0.7\ s^{-1}$, $\tau_t = 60\ s$. Empty circles designate value of R_e, full circles R_s.
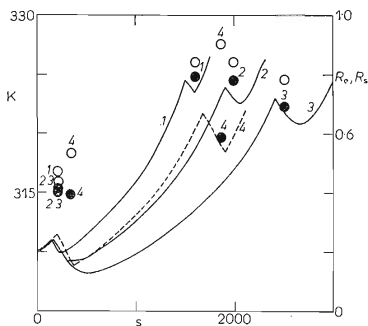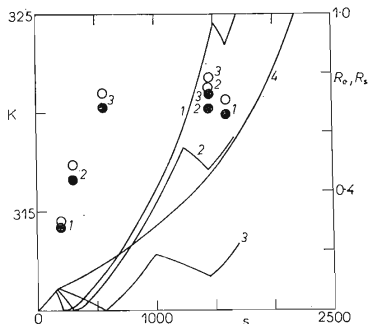

FIG. 2

Start-up of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effect of the flow-rate of the coolant (parameter C) in case of an insignificant thermal capacity of the cooling system: $B = 50$, $\tau_t = 1\ s$; $1\ C = 0.7\ s^{-1}$, $2\ 0.07\ s^{-1}$, $3\ 0.03\ s^{-1}$, $4\ 0.01\ s^{-1}$. The same caption as for Fig. 1

meter B) and the flow rate of the coolant (parameter C) on the reactor start-up are shown in Figs 1 to 3.

Under the conditions of the fast response of the cooling system on the opening of the flow of the coolant, the increased thermal capacity of the cooling system (decreasing B) increases the temperature overshooting after shutting down the cooling system. Although the increased flow rate of the coolant (parameter C) diminishes the temperature overshot after shutting the flow of the coolant, the overregulation of the temperature increases after turning on the cooling system. This effect grows with increasing thermal capacity of the cooling system. This result thus shows that the inertia of the cooling system requires that the temperature of actuation of the cooling system be decreased (Fig. 4).
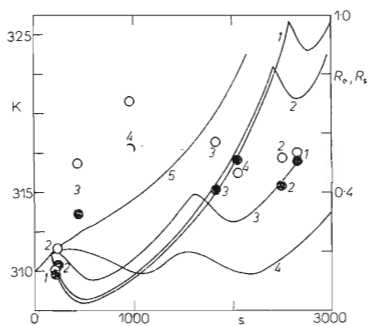

FIG. 3

Start-up of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effect of the flow rate of the coolant in case of a significant thermal capacity of the cooling system: $B = 5$, $\tau_t = 1$ s; 1 $C = 0.7$ s^{-1}, 2 0.07 s^{-1}, 3 0.007 s^{-1}, 4 0.003 s^{-1}, 5 0.001 s^{-1}. The same caption as for Fig. 1

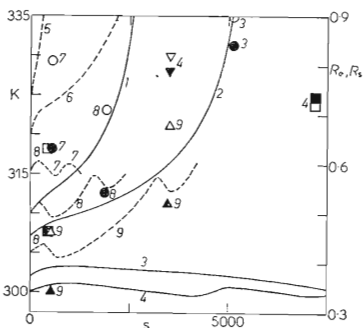

FIG. 4

Start-up of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effect of the initial temperature of the reaction mixture and the coolant: $B = 5$, $\tau_t = 1$ s; 1, 2, 3, 4 $C = 0.001$ s^{-1}, 5, 6, 7, 8, 9 $C = 0.007$ s^{-1}. Empty points designate values of R_e, full points R_s.

The extension of the time for the determination of the degree of utilization R_e.
The inertia of the cooling system thus causes that the effect of turning off or on the
cooling system does not work immediately. As a consequence the system is over-
regulated, the temperature of the reaction mixture overshoots the value $T_{s,n} + T_{reg}$
and after switching off the cooling undershoots the value $T_{s,n} - T_{reg}$. Owing to the
asymmetric behaviour these values of overregulation are not the same. From the
view point of the control the significant fact is that the temperature increase can be
checked quickly by applying a high flow rate of the coolant. The temperature runaway
is the major source of hazard. Under te conditions when the thermal capacity
is large, however, the accompanying phenomenon is the increased "cold" accumulated
in the cooling system and the overegulation of the temperature below the value
$T_{s,n} - T_{reg}$.

A consequence of the inertia of the cooling system is on the one hand the extension
of the necessary time of determination of the experimental value of the degree
of utilization, R_e, and, on the other hand, extension of the time of transition to the
extrapolated value of the temperature of the reaction mixture, $T_{s,n}$. The prolongation
of the time necessary for determination of the degree of utilization, R_e, is influenced
by the inertia of the cooling system both after the switching off and on the cooling.
The extension of this time prolongs the necessary time for acquiring the information
about the instantaneous state of the system, and hence for obtaining the instantaneous
value of the degree of utilization, R_e. This impairs the adaptability of control. For the
reactions, for which the increasing degree of conversion of the reactant the reaction
rate decreases this does not lead to increased hazard. In this case the extension of the
time for the determination of the degree of utilization, R_e, is the source of the ap-
parent decrease of this quantity. The time necessary for the determination of the
extrapolated temperature $T_{s,n}$ is influenced by the inertia of the cooling system after
turning off the cooling; with increased thermal capacity of the cooling system this
time markedly increases.

The extension of the time for the determination of the degree of utilization,
R_e, and the time necessary to reach the extrapolated temperature, $T_{s,n}$, for reactions
of positive order becomes adversely manifest through the decrease of the degree
of utilization, R_e, near the end of the reaction. Examples of this effect are presented
in Figs 5 and 6. It is so because toward the end of the reaction the changes of the
degree of conversion for positive-order reactions play a relatively important role
and because in the extrapolation of the temperature $T_{s,n}$ the effect of the degree
of conversion was neglected[1]. For positive-order reactions it is therefore neces-
sary, in case of decreased catalytic activity in the course of the reaction, to increase
the reaction temperature, Fig. 7. The acumulation of "cold" in the cooling system
extends the time of transition to the extrapolated value $T_{s,n}$ because during this
time the degree of conversion increases, a fact that had not been accounted for
in the simple method of extrapolation. The real degree of utilization. R_s, is therefore

lower than the requested value. The difference between the real and the requested value is the greater the larger the thermal capacity of the cooling system. This means that this phenomenon leads to a certain autoregulation function because the increased thermal capacity of the cooling system automatically decreases the degree of utilization, R_e. This automatically increases the safety of the operation. Unfortunately this automatic mechanism does not provide protection against the increased lag of response of the cooling system due to the decreased flow rate of the coolant, for the decreased flow rate of the coolant diminished the amount of accumulated
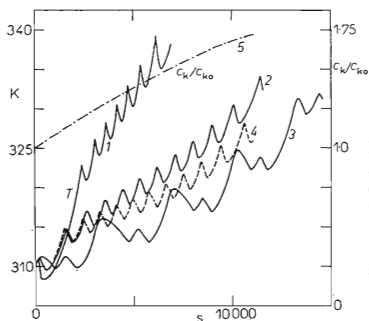

Fig. 5

Examples of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The dependence of the temperature of the reaction mixture on time ($x_k = 0.9$). $B = 5$, $\tau_t = 1$ s; 1 $C = 0.07$ s^{-1}, 2 $C = 0.007$ s^{-1}, 3 0.003 s^{-1}, 4 0.007 s^{-1}, variable catalyst activity, 5 the time dependence of the catalyst activity for the case shown by curve 4
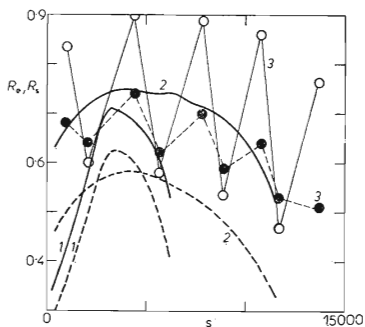

Fig. 6

Examples of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The dependence of the degree of utilization R_e and R_s on time. $B = 5$, $\tau_t = 1$ s; solid lines and empty circles designate the dependence of R_e, broken lines and full circles the dependence of R_s. The remaining caption is the same as for Fig. 5

"cold" in the cooling system and hence cuts short the time for reaching the extrapolated temperature, $T_{s,n}$.

For reactions with autocatalytic kinetics and other cases, when the requirement of constant degree of utilization, R_e, calls for decreased temperature of the reaction mixture, the consequences of the inertia of the cooling system are negative. Also, the risk is increased because during the time of determination of the degree of utilization, R_e, when there is no information about the state of the system, as well as in the course of approaching the temperature $T_{s,n}$, the conditions for controlling the process become less favourable and the information lag increases the risk of failure (Fig. 5 curve 4 and Fig. 8).
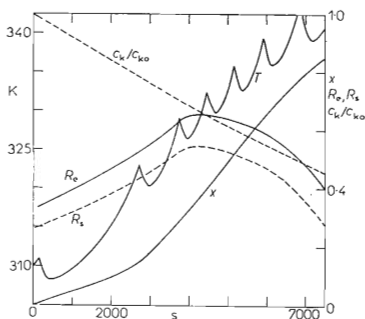

FIG. 7

Example of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effect of the variable catalyst activity ($x_k = 0.9$). $B = 5$, $\tau_t = 1\,s$, $C = 0.07\,s^{-1}$
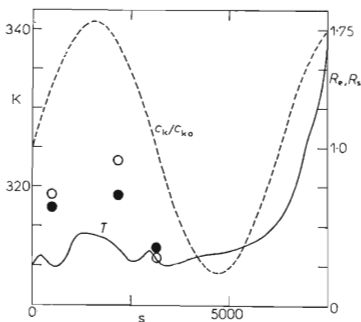

FIG. 8

Example of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effect of variable catalyst activity. $B = 5$, $\tau_t = 1\,s$, $C = 0.007\,s^{-1}$. Empty circles designate the dependence of R_e, full circles R_s

Stability of the Control Algorithm

The used simple method of control neglects in the process of determination of the instantaneous value of the degree of utilization the amount of heat accumulated in the cooling system. It is assumed that at constant value of the temperature of the reaction mixture the accumulation of heat may be neglected. Thus the obtained information is distorted which may eventually lead to an oscillation instability.

After the first actuation of the cooling system the temperature of the system is identical with that of the reaction mixture. At the end of the action of the system the temperature is minimal. By the simplified method of evaluatin of the degree of utilization, R_e, the "cold" accumulated in the cooling system during evaluation is attributed to the chemical reaction, which leads to an apparently higher value of R_e compared to the reality. The consequence is the extrapolation to a lower value of $T_{s,n}$ than would correspond to the given value of the degree of utilization, R_e. Thus the cooling capacity of the system enters the following stage of the process with an accumulated "cold" whose excess is then attributed to a better exchange of heat. Extrapolation of the temperature of the reaction mixture therefore leads to a higher value than would corresponds to the given value of the degree of utilization. The system reaches this value later, the exchange of heat between the reaction mixture and the coolant is more thorough and the coolant enters the next cycle with a low content of accumulated heat and the whole procedure is repeated. An example of such a behaviour of the system is shown in Fig. 5 (curve *3*) and Fig. 6 (curve *3*).
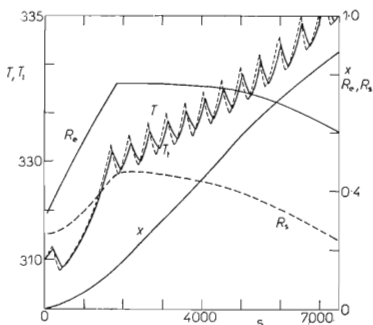

FIG. 9

Example of temperature control in the reaction mixture for a present value of the degree of utilization $R_e = 0.8$. The effect of inertia of the temperature sensor in case of negligible thermal capacity of the cooling system ($x_k = 0.9$). $B = 50$, $\tau_t = 60$ s, $C = 0.7$ s^{-1}. Broken line designates the course of the real temperature of the reaction mixture ($\tau_t = 1$ s)

The Inertia of the Sensor Detecting the Temperature of the Reaction Mixture

This inertia brings along similar consequence as the inertia of the cooling system, with the difference that the inertia of the temperature sensing device is symmetric. However, even this symmetric inertia may have an asymmetric result as it triggers into the action the inertia of the cooling system. An example of the inertia of the sensor in case of a fast response of the system to a control action is shown in Fig. 1 (curve *4*) and Fig. 9. The presented method of control of temperature of the reaction mixture provides to some extent an automatic safeguard against the deterioration of the dynamic properties of the sensor, for the increased inertia of the sensor brings along an automatic decrease of the degree of utilization, R_e.

The results of the simulation have shown that the proposed method of control of the temperature of the reaction mixture is applicable even for reactors with a large inertia of the cooling system. For reactions with decreasing demand for the exchange of heat in the progress of the reaction the application is safe. For reactions for which the demand on the cooling increases with the degree of conversion (autocatalytic reactions, reactions leading to increased viscosity of the reaction mixture, fouling of the heat exchange surface) the inertia of the cooling system poses a serious threat to the safety of the operation.

LIST OF SYMBOLS

$A = k_h P/(V c_p \varrho)$	parameter of system characterizing intensity of heat exchange between the reaction mixture and the cooling system (s^{-1})
B	parameter defined by Eq. (2)
C	parameter defined by Eq. (3) (s^{-1})
c_{A0}	initial concentration of reactant $(kmol/m^3)$
c_k, c_{k0}	concentration of catalyst in the reaction mixture, initial concentration $(kmol/m^3)$
c_p, c_{pc}	specific heat of the reaction mixture and coolant $(kJ/kg\ K)$
k_h	heat transfer coefficient $(kW/m^2\ K)$
P	exchange area of heat exchange surface (m^2)
R_e	instantaneous value of the degree of utilization of the cooling capacity of reactor (Eq.) (*1*)
R_s	real value of the degree of utilization of cooling capacity
r	reaction rate $(kmol/m^3\ s)$
T	temperature of the reaction mixture (K)
T_c	temperature of coolant in the cooling system (K)
T_{ci}	inlet temperature of coolant (K)
T_0, T_{c0}	initial temperature of mixture and coolant (K)
$T_{s,n}$	temperature of the reaction mixture corresponding to the present value of the degree of utilization of the cooling capacity (K)
T_{reg}	width of hysteresis band of controller (K)
T_t	temperature of the mixture measured by the sensor (K)
t	reaction time (s)

t_a	time of idling of the cooling system in the course of determination of R_c (s)
t_c	time of operation of the cooling system in the course of determination of R_c (s)
V, V_c	volume of reaction mixture and coolant (m^3)
x, x_k	degree of conversion of reactant and its final value
ΔT_{ad}	adiabatic temperature rise (K)
ϱ, ϱ_c	density of the reaction mixture and the coolant (kg/m^3)
τ_t	time constant of temperature sensing device (s)

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