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CONTROL OF CHEMICAL REACTOR FOR CONSECUTIVE REACTION I

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A new strategy for the control of the continuous stirred tank reactor (CSTR) with a consecutive reaction is presented. The new control strategy - the self-tuning controller is derived from the reactor behaviour in both the steady - and the transient states. The controller is briefly described and results of simulation calculations are presented.

Introduction

There are some processes in chemical industry that exhibit a response which is referred to as "inverse response". The transfer function that describes this type of response requires a positive zero

$$F_s = \frac{K(1 - \tau_1 s)}{(\tau_2 s + 1)(\tau_3 s + 1)}$$

This type of system is usually nonlinear and, therefore, the parameters K, τ_1, τ_2 and τ_3 are sensitive to operating conditions.

One of such processes is CSTR producing substance B in a consecutive reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

In such situations cascade and feedforward control schemes are usually used to improve the performance provided by feedback control[1].

Mathematical Model of CSTR

Let have a consecutive reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ where A is an input component, B is a desired product and C is a waste product. The main task of the process is to reach the maximum concentration of the product B and this task has to be fulfilled in spite of different disturbances. The steady-state analysis gives the following relation for the concentration of the component B i.e. x_B:

$$x_B = \frac{\tau k_1 x_{A0}}{(1+\tau k_1)(1+\tau k_2)} \tag{1}$$

where $\tau = V/Q$

V - reactor volume

Q - input flow to the system

x_{A0} - intput concentration of the component A

k_1, k_2 - rate constants of reactions

$$k_1 = 10^9 \exp\left[-\frac{6000}{T}\right] \qquad k_2 = 10^{13} \exp\left[-\frac{9000}{T}\right] \tag{3}$$

constants k_1 and k_2 have been taken from the literature)

T - temperature, K

It can be seen from Eq. (1) that the concentration x_B depends on the value τ (i.e. on the volume flow) and on the reaction rate constants k_1 and k_2 (i.e. on temperature).

Figure 1 shows the graph $x_B = f(\tau)$ for temperatures 20 °C, 50 °C and 80 °C. All steady state characteristics exhibit the maximum. Owing to the fact that the gain of the system approaches zero in the region of maximum concentration x_B, we must be satisfied with suboptimal control only. For such a situation the working point of the reactor lies on the rising side of the characteristic. It follows from Fig. 1 that the temperature increase results in:

a) "tapering" of the steady state characteristic curve

b) "lowering" of the maximum value of x_B

c) "shifting" of the maximum value of x_B to the higher values of the flow.

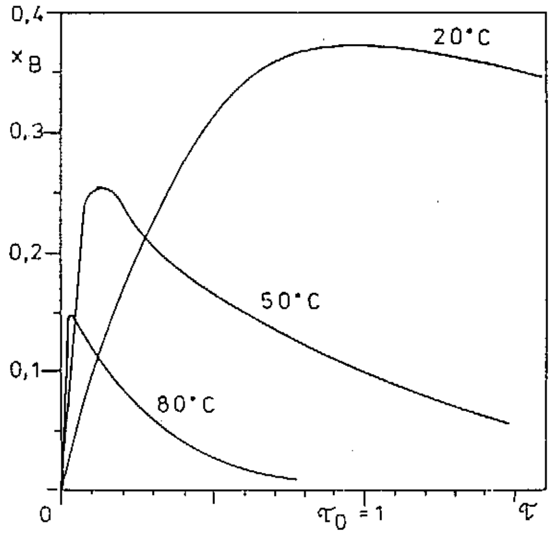

Fig. 1 Steady - state behaviour of the CSTR

The "tapering" of the steady-state characteristic curve for a given value of the flow produces an increase in the reactor gain and the "lowering" of the maximum value of x_B produces, on the contrary, a decrease in the reactor gain.

It is known that the dynamic behaviour of the CSTR can be described by a second- order transfer function (see e.g. Ref.[2]). A sampling period significantly affects the behaviour of the CSTR. That means that the system can be classified as a system with the minimum or the nonminimum phase. This fact has to be taken into account in the selection of a control algorithm.

Control Strategy for the CSTR

The CSTR is a nonlinear system, simplified in the first approach to a single-input, single-output (SISO) system. The system is, in the close surrounding of the operating point, approximately linear. Its input variable is τ (the function of the flow, see Eq. (2) and output variable is the concentration x_B. The dynamic behaviour of the reactor can be influenced in an unfavourable way by disturbances produced mainly by changes in:

- temperature of the reaction
- system parameters
- variable τ i.e. volume flow Q.

Let suppose that the CSTR is controlled by a concentration controller. With respect to the changes of the static parameters, let consider the implementation of an adaptive controller. The controller has to ensure the on-line identification of the CSTR dynamics and the breakdownless closing of the control loop.

Another task that has to be ensured is a reasonable response of the closed loop in the case of changes in the system behaviour e.g. for the operating point changes, disturbances in the volume flow or for changes of system parameters. Such changes can be caused by disturbances in the reactor temperature, the quality of the feed etc.

Brief Description of the Concentration Controller

To fulfil all the given tasks we can use a self-tuning controller (STC) - Fig. 2. We assume that the CSTR can be described by the difference equation[3]

$$\Delta y(k) + a\Delta y(k-1) = b_1\Delta u(k-1) + b_2\Delta u(k-2) + b_3\Delta u(k-3) + e(t) \tag{4a}$$

where

$$\Delta u(k) = u(k) - u(k-1) \tag{4b}$$

$$\Delta y(k) = y(k) - y(k-1) \tag{4c}$$

and $e(t)$ is a stochastic noise variable with the normal distribution, the zero mean and the finite variance.

The on-line identification is realized by the recursive least-square method. The numerical stability of the identification algorithm is ensured by the known LD decomposition of the variable matrix. The on-line estimation of the CSTR

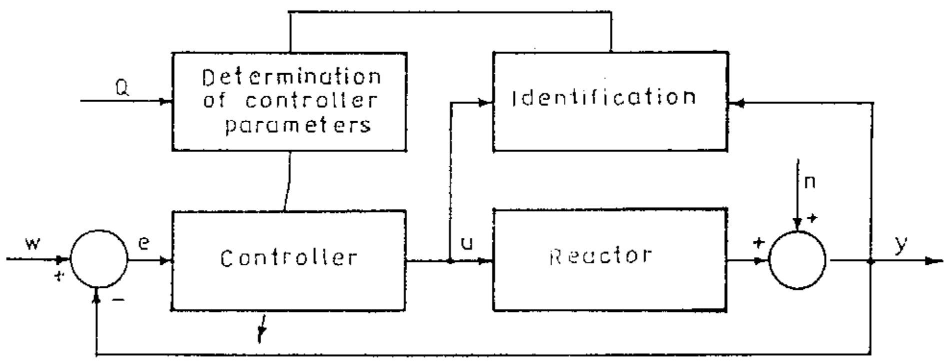

Fig. 2 Closed control loop with STC

parameters is supplied by the restricted exponential forgetting[4]. The estimation of parameters is realized by the subroutine REDIC[5], 1985). The controller equation is based on the modern polynomial method, the control loop stability is ensured for the case of nonminimum phase system as well.

The controller is designed to minimize the criterion Q (Ref.[3]).

$$Q = \lim_{T_k \to \infty} \frac{1}{T_k} E\left\{\sum_{k=1}^{T_k} [y(k) - W]^2 + h[\Delta u(k)]^2\right\} \tag{5}$$

where $u(k)$ - manipulated variable (corresponding to the value τ)

$y(k)$ - controlled variable (corresponding to the concentration x_B)

W - required value of the controlled variable

h - penalty constant (enables the lowering of the manipulated variable variance)

T_k - the so-called control horizont

The controller equation is

$$u(k) = \delta^{-1}\{r_1\Delta u(k-1) + r_2\Delta u(k-2) + s_1[y(k) - W] + s_2[y(k-1) - W]\} \tag{6}$$

here r_1, r_2, s_1, s_2, δ are controller coefficients solved in each control step by the subroutine FAKTR[3].

Simulation of the Control

The CSTR is simulated on a digital computer by means of two transfer elements (Fig. 3):

- the nonlinear element describes the steady-state behaviour of the CSTR

$$y_u = S_1 + S_2(u - p_0)^2 \tag{7}$$

where u corresponds to the value τ (in Fig. 1), y_u to the concentration x_B in the steady-state and the parameters S_1, S_2 and p_0 simulate the shape, the shift and the maximum value of the steady-state characteristic.

- the linear element describes the dynamic behaviour of the CSTR in operating point by the transfer function

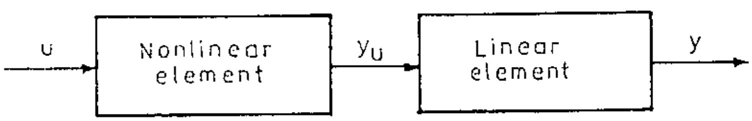

Fig. 3 The model of the CSTR

$$F(p) = \frac{Y(p)}{Y_u(p)} = \frac{1 - pT_1}{(1 + pT_2)(1 + pT_3)} \quad (8)$$

Depending on the sampling interval the CSTR operates either like a minimum or a nonminimum phase system.

The relation (7) approximates the function $x_B = f(\tau)$ for T = 20 °C (see Fig. 1) in its rising part and it has the following parameters

$$y_u = 0.375\,[1 - (u - 1)^2] \quad (9)$$

The time constants of the transfer function (8) were T_1 = 4 time units, T_2 = 4 time units and T_3 =10 time units. For the sampling interval T = 8 time units the reactor behaviour corresponds to the nonminimum and for T = 16 time units to the minimum phase system. The resulting difference equations are
For T = 8

$$y(k) - 0.5846\,y(k-1) + 0.0608\,y(k-2) = 0.132\,u(k-1) + 0.3441\,u(k-2) \quad (10)$$

For T = 16

$$y(k) - 0.2202\,y(k-1) + 0.0037\,y(k-2) = 0.5533\,u(k-1) + 0.3441\,u(k-2) \quad (11)$$

Our control algorithm was always started with the following parameters:
1. Initial values of parameters $\hat{\gamma}_i$ in Eq. (4a): $\hat{\gamma}_i = 0$ for $i = 1,\ldots, 4$.
2. The penalty constant h in the criterion (5): h = 1. The value h = 1 was accepted owing to the fact, that for the stability of a control loop is needed $h \geq 0.5$ needed.
3. Initial values of controller parameters Eq. (6): $r_1 = r_2 = s_1 = s_2 = 0$; $\delta = 1$.

Simulation experiments were performed for several practical situations and the simulation results are shown for the nonminimum phase system (i.e. T = 8) with a significantly low additive noise at the system output. In simulation experiments we tested, first of all, the tuning of the reactor operating point for normal working conditions and, at the same time, the identificational part of the control algorithm. Simulation tests were completed by a check to find out whether in the case of the control loop closing occur any inadmissible changes of the control loop quantities. In the case of open loop the input signal is u = 0.635 and the controlled variable is to reach the desired value y_u = 0.325 in the steady state (see point P_1 in Fig. 4.).

In the course of reaching the working point the process identification is produced. The control loop is closed in the 10[th] step. The time dependence of system output variable, the model parameters and the exponential forgetting coefficient are shown in Fig. 5.

In about five steps of the identification process the system response and model parameters are stabilized. The control loop closing is breakdownless i. e.

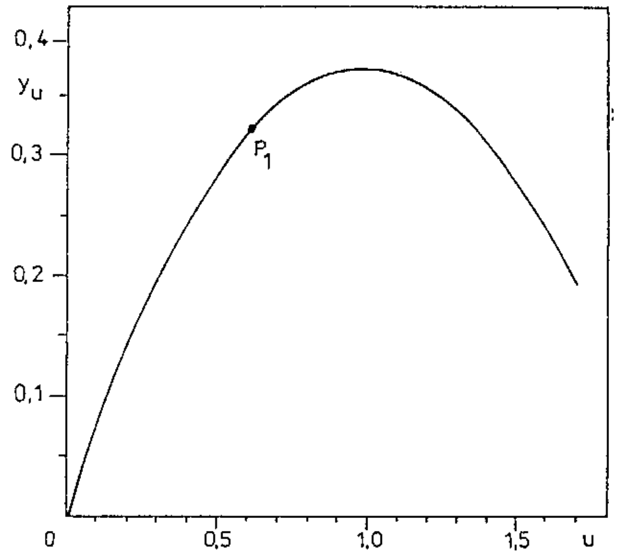

Fig. 4 Steady-stade characteristic curve of the CSTR model

without remarkable overshoot in controlled and manipulated variables. The steady-state error of the control loop is always zero.

The above-mentioned experiments create a basis for many other calculations. The aim of the following calculations will be a check of how the described control algorithm will operate in the presence of both disturbances entering the control loop and changes in reactor parameters.

Conslusion

The present papers shows that the CSTR can be taken as a system changing its response according to the reactor temperature and input material properties.

The described system behaves as a system with the minimum or nonminimum phases. This depends on the value of the sampling interval. The control of the described reactor is performed by a self-tuning controller with the penalty of the manipulated variable, the restricted exponential forgetting digital filtration is used for the numerical stability of the algorithm.

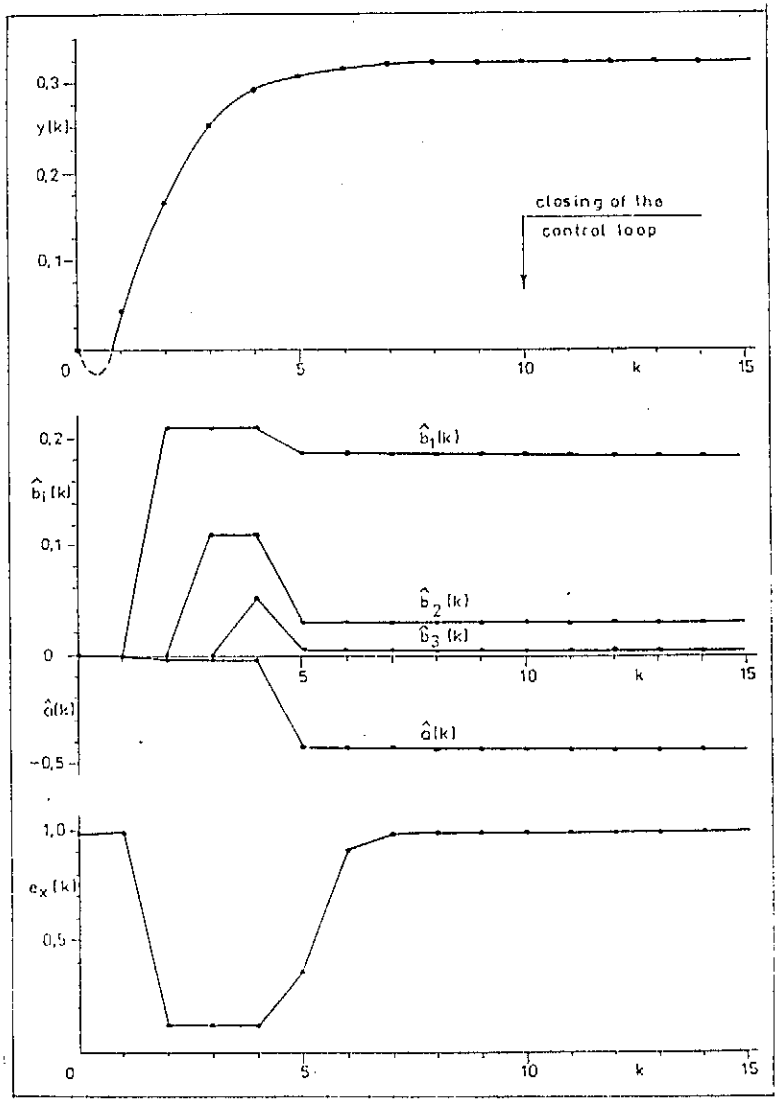

Fig. 5 Time dependence of system output variable, model parameters and the exponential forgetting

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