Unstable Suboptimal Periodic Control of a Certain Chemical Reactor

MASAKAZU MATSUBARA AND KATSUAKI ONOGI

Abstract—**The suboptimal periodic control of a CSTR (continuous stirred tank reactor) in which two reactions are occurring in parallel is sought by use of a computer simulation technique. The results indicate that the corresponding suboptimal periodic state may be unstable under open-loop control and, consequently, some stabilization technique which will be proposed in another work is required. Structure analysis based on the stroboscopic approach is successfully applied for determining the periodic state which might be unstable.**

I. Problem Description

Suppose that two irreversible, exothermic reactions $A \to B$ and $A \to C$ of the αth order and of the first order, respectively, are taking place in a CSTR equipped with a jacket or a coil to which a coolant is fed for temperature control. The products B and C are the desired product and the waste product, respectively. The state equation can be written as

$$\dot{x}_1 = 1 - x_1 - ae^{-\epsilon/x_3}x_1^{\alpha} - be^{-\rho\epsilon/x_3}x_1 \tag{1a}$$

$$\dot{x}_2 = -x_2 + ae^{-\epsilon/x_3}x_1^{\alpha} \tag{1b}$$

$$\dot{x}_3 = \lambda_1 ae^{-\epsilon/x_3}x_1^{\alpha} + \lambda_2 be^{-\rho\epsilon/x_3}x_1 - (x_3 - \theta_c)u - (x_3 - \theta_f) \tag{1c}$$

where

$$0 < x_1 < 1, \quad 0 < x_2 < 1, \ x_3 > 0, \ u > 0, \ \theta_c > 0, \ \theta_f > 0 \tag{2}$$

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The authors are with the Department of Chemical Engineering, Nagoya University, Nagoya, Japan.

lanuscript received August 28, 1978.
he author is with the University of California at Davis, Davis, CA 95616.

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and a, b, α, ϵ, ρ, λ_1, and λ_2 are parameters with positive values. The x_1 and x_2 are the normalized concentrations of A and B, respectively, while the x_3, θ_c, and θ_f are the normalized temperatures of reactor content, coolant feed, and raw material feed (A only), respectively. The u which is proportional to the overall heat transfer coefficient can be adjusted by changing the coolant flow rate. When the reactor is subject to a periodic control with period τ satisfying the constraint

$$u_* \leq u \leq u^*, \tag{3}$$

it is assumed that there exists at least one periodic state (or periodic regime) with period $m\tau$, $m=1,2,\cdots$ such that

$$x_1(0)=x_1(m\tau), \quad x_2(0)=x_2(m\tau), \quad x_3(0)=x_3(m\tau). \tag{4}$$

Then, it is desired to maximize the average yield of B

$$J(u)=\frac{1}{m\tau}\int_0^{m\tau} x_2\,dt \tag{5}$$

subject to the conditions (1)–(4), where the value of m will, in most cases, be equal to one.

The above optimal periodic control problem has already been studied in detail [1] for the case of θ_f lower than θ_c. Although such a case seems unusual, the resulting optimal periodic state is usually stable. In this paper the case of θ_f higher than θ_c is studied and it is observed that the optimal periodic state is apt to be unstable in such a situation. Since the general analytical solution of our problem is impossible, only some numerical solutions are sought. Structure analysis based on the stroboscopic approach [2] which has recently been proposed by the present authors is used for determining the existence and location of periodic states which might be unstable.

The optimal steady control of the above problem, $\bar{u}^\circ$, is an internal control such that $u_*<\bar{u}^\circ<u^*$ if and only if the condition

$$\alpha\rho>1 \tag{6}$$

is satisfied in addition to a suitable choice of u_* and u^* [1]. When $\bar{u}^\circ$ is an internal control, the optimal periodic control must be proper if the condition

$$\rho<1 \tag{7}$$

is satisfied [1]. Since our interest is only in the case of the optimal periodic control being proper, the values of parameters and control bounds were so chosen as to satisfy these conditions. They are

$$\alpha=2, \quad \rho=0.85, \quad a=10^2e^{28}, \quad b=10^2e^{23}, \\ \epsilon=10^2, \quad \lambda_1=1.0, \quad \lambda_2=1.2 \tag{8}$$

and

$$u_*=0.0 \quad \text{and} \quad u^*=5.0, \tag{9}$$

respectively. The feed conditions satisfying $\theta_f>\theta_c$ were chosen as

$$\theta_f=2.7, \quad \theta_c=2.5. \tag{10}$$

The optimal steady control can easily be determined as

$$\bar{u}^\circ=0.5534. \tag{11}$$

There exist three singular points (equilibrium states) and no limit cycle in the state space of the reactor, subject to the optimal steady control (11). The singular points are a stable node, a stable focus, and a saddle. The optimal steady state corresponds to the saddle for which

$$J(\bar{u}^\circ)=0.1917. \tag{12}$$

II. Suboptimal Periodic Control

It is known that the optimal periodic control must be a bang-bang control under the conditions $u_*<\bar{u}^\circ<u^*$ and (7) [1]. So, we assume the type of the optimal periodic control as

$$u(t)=\begin{cases} u^*, & k\tau<t<(k+\sigma)\tau \\ u_*, & (k+\sigma)\tau<t<(k+1)\tau, \end{cases} \qquad k=\cdots,-1,0,1,\cdots;\ 0<\sigma<1 \tag{13}$$

and seek the values of τ and σ which maximize the value of $J(u)$ in (5) subject to (1), (2), and (4). The sought control will be suboptimal with respect to the original optimal periodic control problem because a bang-bang control with more frequent switching in each period may be optimal.

Now, our problem reduces to a nonlinear programming problem with two decision variables, τ and σ which are constrained in a band-shaped area

$$\{(\tau,\sigma)|0<\tau<\infty \text{ and } 0<\sigma<1\}. \tag{14}$$

Care must, however, be taken about the fact that $J(u)$ is in general a many-valued function of τ and σ because there can exist many periodic states corresponding to a specific control. In addition, some periodic state may be unstable. So, it will not be so easy to determine accurate optimal values of τ and σ. To help smooth determination of these values, the contour map of $J(u)$ in the $\tau\sigma$-plane will in the first step be roughly anticipated from the value of $J(u)$ at the boundary of (14) which can easily be determined. Similar technique has recently been used by Sinčić and Bailey [3], [4].

At the boundaries $\sigma=0$ and $\sigma=1$ of (14) the bang-bang control (13) reduces to the steady controls $\bar{u}=u_*=0$ and $\bar{u}=u^*=5.0$, respectively. It is easy to show that there exists for each of these steady controls a unique singular point being a stable node and no limit cycle. The value of $J(u)$ becomes 0.009504 for $\bar{u}=u_*$ and 0.001044 for $\bar{u}=u^*$. At the boundary $\tau\to\infty$ the state of the reactor tends to the stable nodes corresponding to $\bar{u}=u^*$ and $\bar{u}=u_*$ in the interval $k\tau<t<(k+\sigma)\tau$ and $(k+\sigma)\tau<t<(k+1)\tau$, respectively. Hence, there appears a unique quasi-steady state for which the value of $J(u)$ is equal to $\sigma J(u^*)+(1-\sigma)J(u_*)$ $=0.009504-0.008460\sigma$. At the remaining boundary $\tau=0$, the bang-bang control reduces to a relaxed control in which the value of u is switched infinitely fast between u^* and u_* at the time ratio of σ to $1-\sigma$. It is known for a system being linear with respect to u as in (1) that a steady control $\bar{u}=\sigma u^*+(1-\sigma)u_*=5\sigma$ is equivalent to such a relaxed control. So, there exist relaxed singular points and relaxed limit cycles for the relaxed control which just agree with singular points and limit cycles for the corresponding steady control. Along these lines it can be ascertained that there exist three relaxed singular points for $0.003870<\sigma<0.1164$ and a unique relaxed singular point for $0<\sigma<0.003870$ and $0.1164<\sigma<1$ and that there exists no relaxed limit cycle for $0<\sigma<1$. In the interval of σ having three relaxed singular points the value of $J(u)$ is maximal for the relaxed singular point of the saddle mode and a jump in the maximal value of $J(u)$ occurs at two extremes of that interval.

If the value of τ is increased from zero to infinity for a fixed value of σ in the interval $0.003870<\sigma<0.1164$, the number of periodic states must change from three to one at a certain value of τ because the number is equal to three and one for $\tau=0$ and $\tau\to\infty$, respectively. On the other hand, if the fixed value of σ does not belong to the above interval, the change in the number of periodic states will not necessarily occur because the number is equal to one for both $\tau=0$ and $\tau\to\infty$. These considerations suggest that there exists a curve dividing the region in (14) into two subregions where the number of periodic states is equal to one and three, respectively, and that the two ends of the curve are lying at the points corresponding to $\sigma=0.003870$ and 0.1164 on the line $\tau=0$. Further, the contour map of $J(u)$ in the $\tau\sigma$-plane will indicate a fault line just along that curve. Also, it is likely that the maximal value of $J(u)$ will occur within the subregion inside the fault line.

Keeping the above-stated points in mind, a rough contour map of $J(u)$ was made out as shown in Fig. 1. This map indicates that the optimal point is certainly lying in the subregion inside the fault line and that the map is unimodal within the subregion. Based on these observations, more accurate determination of the optimal point was attempted by applying the complex method [5] to a small rectangular region including the forecasted optimal point. The resulting optimal point is given by

$$\tau=0.8874 \quad \text{and} \quad \sigma=0.1053. \tag{15}$$

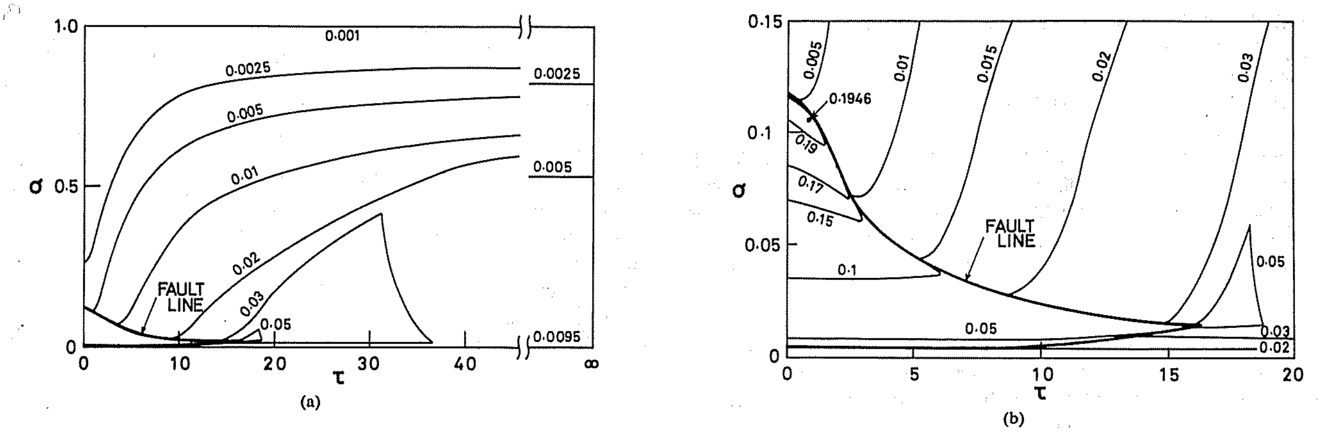

Fig. 1. Contour map of $J(u)$ in $\tau\sigma$-plane. (a) The entire picture. (b) Details of the subregion inside the fault line.

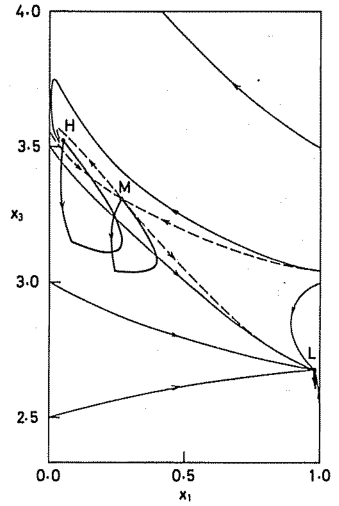

Fig. 2. The equiphase trajectories and the periodic states for the optimal periodic control ($\tau=0.8874$ and $\sigma=0.1053$). L: Stable node, $J(u)=0.005500$; M: Saddle, $J(u)=0.1946$; H: Stable focus, $J(u)=0.1656$.

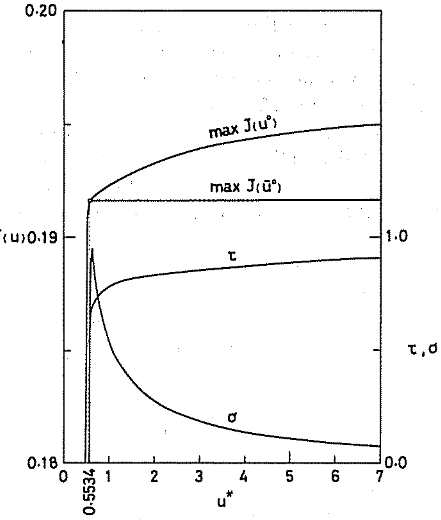

Fig. 3. The maximal values of $J(u)$ for the optimal periodic control and the optimal steady control versus the value of u^* (the value of u_* is fixed at zero).

In the state equation (1) the x_2 is included only in (1b) and in the consequence the system behavior in the x_1x_3-space is not dependent on the x_2. The equiphase trajectories [2] in the x_1x_3-space corresponding to the optimal bang-bang control in (15) are depicted in Fig. 2. The trajectories are determined for the phase when the control is switched from u_* to u^*. The discrete equiphase system has three discrete singular points L, M, and H corresponding to three periodic states of the original system which are also indicated in Fig. 2. Stability analysis [2] indicates that these discrete singular points or the corresponding periodic states are a stable node, a saddle, and a stable focus, respectively. The values of $J(u)$ for these points are 0.00550, 0.1946, and 0.1656, respectively, and therefore the periodic state of the saddle mode corresponding to the point M is optimal. The value of $J(u)$ is improved by about 1.5 percent relative to the value in (12) corresponding to the optimal steady control in (11).

To illustrate the change in the optimal point due to change in the control bounds, the values of $J(u)$ for the suboptimal periodic control and the optimal steady control versus the value of u^* are indicated in Fig. 3. In the interval of u^* less than $\bar{u}^\circ$ in (11), the optimal periodic control is not proper but a steady boundary control $\bar{u}=u^*$. The suboptimal periodic state or the optimal steady state is of the saddle mode for $0.01935<u^*<\infty$ and of the stable nodal mode for $0<u^*<0.01935$.

III. Concluding Remarks

The suboptimal periodic state of the reactor corresponding to the suboptimal periodic control is apt to be unstable under the usual feed condition such that $\theta_f>\theta_c$ and, in addition, it may be of the saddle mode. Use of the structure analysis based on the stroboscopic approach is not only indispensable for finding a periodic state of the saddle mode but also useful for determining the optimal periodic state under the existence of multiple periodic states.

Stabilization of the unstable optimal periodic state will be proposed in another work [6].

References

[1] M. Matsubara, Y. Nishimura, and N. Takahashi, "Periodic operation of CSTR-II practical control," *Chem. Eng. Sci.*, vol. 28, pp. 1379–1385, July 1973.

[2] M. Matsubara and K. Onogi, "Structure analysis of periodically controlled nonlinear systems via stroboscopic approach," *IEEE Trans. Automat. Contr.*, vol. AC-22, pp. 678–680, Aug. 1977.

[3] D. Sinčić and J. E. Bailey, "Transient and periodic phenomena for forced cycling of parallel reactions in an adiabatic CSTR," presented at 4th Internat./16th European Symp. Chem. Reaction Engng, Apr. 1976, Heidelberg, Germany.

[4] ——, "Pathological dynamic behavior of forced periodic chemical processes," *Chem. Eng. Sci.*, vol. 32, pp. 281–286, 1977.

[5] M. J. Box, "A new method of constrained optimization and a comparison with other methods," *The Comput. J.*, vol. 8, no. 1, pp. 42–52, 1965.

[6] M. Matsubara and K. Onogi, "Stabilized suboptimal periodic control of a chemical reactor," this issue, pp. 1005–1008.