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PARAMETER–SPACE CLASSIFICATION OF THE DYNAMIC BEHAVIOR OF THE CHEMOSTAT SUBJECT TO PRODUCT INHIBITION

Y. LENBURY,[a] S. ROONGRUANGSORAKARN[b] AND N. TUMRASVIN[a]

a) *Department of Mathematics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.*

b) *Department of Mathematics and Computer Sciences, Faculty of Applied Science, King Mongkut's Institute of Technology, North Bangkok, Bangkok 10300, Thailand.*

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ABSTRACT

Agrawal[1] and later Suzuki[2] have recently classified the dynamic behavior of a continuous microbial flow reactor employing, respectively, the two and three parameter substrate inhibition model. In this report we use the two variable product inhibition model proposed by Yano and Koga[3] with a modified specific growth rate and derive the boundary equations which divide the parameter space of different dynamic behavior.

INTRODUCTION

Ever since the papers of Poore (1973) and Uppal[4] on bifurcation theory and its application to the investigation of periodic behavior of well-stirred chemical reactors, much work has been done in a similar attempt on biochemical reactors. Such oscillatory behavior have been frequently observed in both batch and continuous biological systems (Bonomi[5] and Borzani[6]) and many models have been developed to analyse their dynamic behavior. Variation of the yield term (Y) by Agrawal[1] and Crooke,[7] has led to damped and sustained oscillations, respectively, in a continuous culture. Similar investigation on a batch culture was made by Lenbury,[8] where a simple set of ordinary non-linear differential equations based on the Monod model was utilized.

Here, we shall examine a simple product inhibition model of a continuous-stirred tank reactor proposed by Yano and Koga[3] and derive the boundary equations which completely divide the parameter space of different dynamic behavior.

SYSTEM MODEL

In the case where the growth-limiting substrate (S) is supplied in sufficient amount so that at any moment the concentration change of S has little affect on the dynamic behavior of the system, the single-vessel continuous fermentation system can be described by the following two-variable system:

$$\frac{dX}{dt} = \mu(P)X - DX \tag{1}$$

$$\frac{dP}{dt} = \frac{\mu(P)X}{Y} - DP, \tag{2}$$

where X represents the cells concentration ; P the ethanol concentration ; $\mu(P)$ the specific growth rate ; Y the cells to product yield ; and D the dilution rate.

Following the work of Lenbury and Chiaranai,[9] we consider here the yield coefficient of the form

$$Y(P) \equiv c - dP, \tag{3}$$

where c and d are positive constants. Also, we consider the following modified form of the specific growth rate ;

$$\mu(P) \equiv \frac{\mu_m(1 - P/K_1)}{(K_p - P)} , \tag{4}$$

which is a combination of the Monod's model and that proposed by Yano and Koga. Here, we assume that K_1 and K_p are positive constants. Fig.1 shows plots of $\mu(P)$ and $\sigma(P) = \mu(P)/Y(P)$ for suitable parametric values. Although other more general forms may be used for these functions, it can be shown that (3) and (4) are enough to describe limit cycles and their stability which are to be investigated.

Introducing a new set of variables, namely ; $x_1 \equiv X/dY(0)$, $x_2 \equiv P/K_1$, $\tau \equiv Dt$, $D_0 \equiv \mu(0)/D$, $M(x_2) \equiv \mu(K_1x_2)/\mu(0)$, $y(x_2) \equiv Y(K_1x_2)/Y(0)$, $\alpha \equiv K_p/K_1$, $\beta \equiv c/dK_1$,

the Eqs. (1) through (4) become

$$\frac{dx_1}{d\tau} = (D_0M(x_2) - 1)x_1 \tag{5}$$

$$\frac{dx_2}{d\tau} = -x_2 + D_0M(x_2)x_1/y(x_2) \tag{6}$$

$$M(x_2) = \frac{\alpha(1 - x_2)}{\alpha - x_2} \tag{7}$$

$$y(x_2) = (\beta - x_2)/\beta \, . \tag{8}$$

In order that $M(x_2)$ and $\Sigma(x_2) \equiv M(x_2)/y(x_2)$ have positive function values for x_2 on (0,1), we assume that $\alpha \geqslant 1$ and $\beta \geqslant 1$.

STABILITY OF STEADY STATES

The steady state solutions are obtained from Eqs. (5) and (6) as

(a) trivial solution (washout) : $\bar{x}_1 = \bar{x}_2 = 0$.

(b) nontrivial solution (s) : $\bar{x}_1 = y(\bar{x}_2)\bar{x}_2$, $M(\bar{x}_2) = 1/D_0$ where $(\bar{\ })$ indicates steady state.

Let J be the Jacobian matrix of Eqs. (5) and (6) evaluated at the steady state of interest,

$$J = \begin{bmatrix} -1 + D_0M(\bar{x}_2) & D_0M'(\bar{x}_2)\bar{x}_1 \\ D_0\,\Sigma(\bar{x}_2) & -1 + D_0\,\Sigma'(\bar{x}_2)\bar{x}_1 \end{bmatrix} \tag{9}$$

where the prime denotes differentiation with respect to x_2. The necessary and sufficient conditions for local stability of a steady state are that the eigenvalues have negative real parts, which are equivalent to

$$\det J > 0 \text{ and } \operatorname{tr} J < 0. \tag{10}$$

It follows that the washout steady state is a stable node for $D_0 < 1$ and a saddle point (unstable) for $D_0 > 1$.

For the nontrivial steady states,

$$\det J = -D_0M'(\bar{x}_2)\bar{x}_2 \tag{11}$$

and

$$\operatorname{tr} J = -1 + \Sigma'(\bar{x}_2)\bar{x}_2/\Sigma(\bar{x}_2). \tag{12}$$

Hence, the necessary and sufficient conditions for local stability are

$$M'(\bar{x}_2) < 0 \tag{13}$$

and

$$\Sigma'(\bar{x}_2) < \Sigma(\bar{x}_2)/\bar{x}_2. \tag{14}$$

BIFURCATION OF LIMIT CYCLES

The Hopf–bifurcation occurs when J has pure imaginary eigenvalues, namely

$$\det J > 0 \text{ and } \operatorname{tr} J = 0. \tag{15}$$

For the nontrivial steady states the condition (15) becomes

$$M'(\bar{x}_2) < 0 \tag{16}$$

and

$$\Sigma'(\bar{x}_2) = \Sigma(\bar{x}_2)/\bar{x}_2. \tag{17}$$

TABLE 1 Typical phase – plane plots

CASE	A	B	C	D
Stable washout (node)	1	0	0	0
Unstable washout (saddle point)	0	1	1	1
Stable normal (node or focus)	0	1	0	1
Unstable normal (node or focus)	0	0	1	0
Stable limit cycle	0	0	1	1
Unstable limit cycle	0	0	0	1
Total invariants	**1**	**2**	**3**	**4**

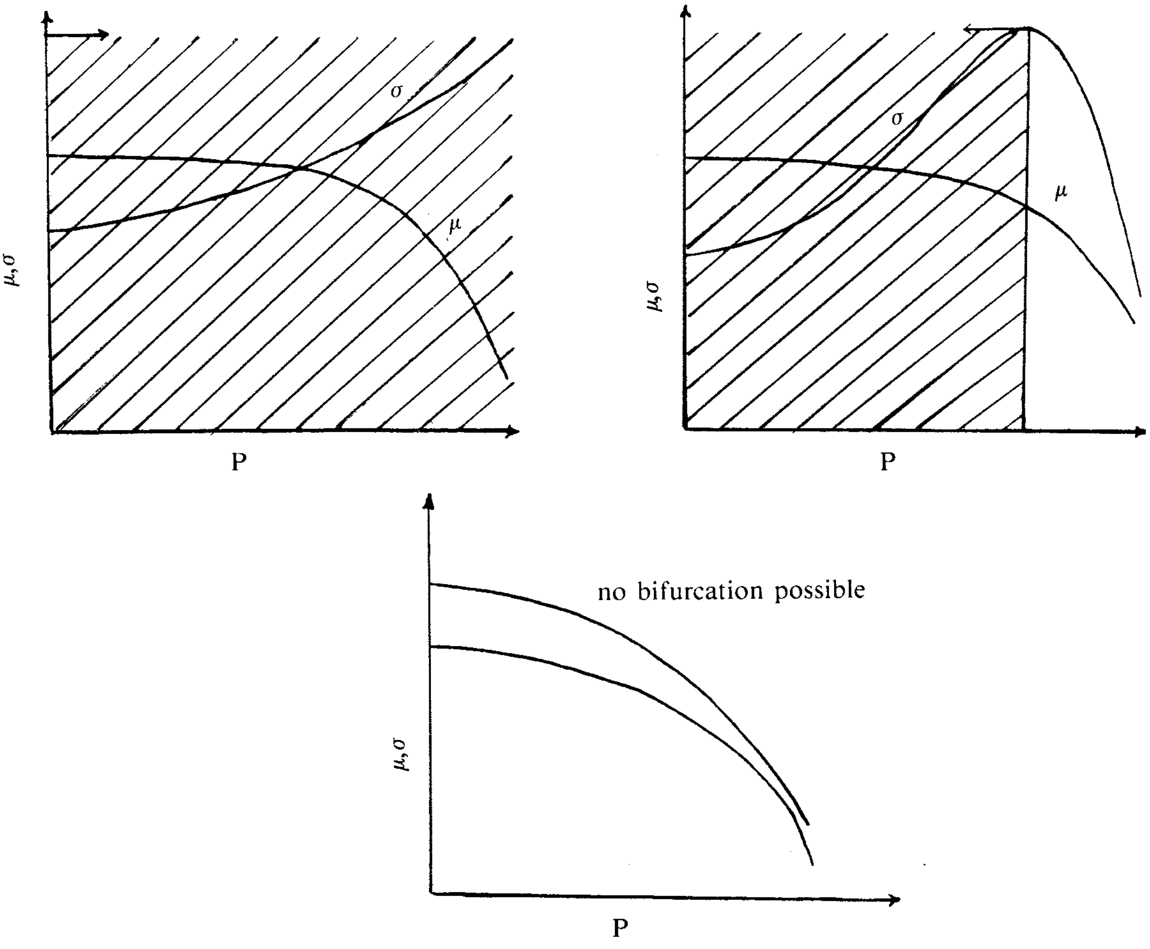

Fig. 1 Plot of typical μ and σ curves. Shaded portion indicates possible regions of bifurcation.

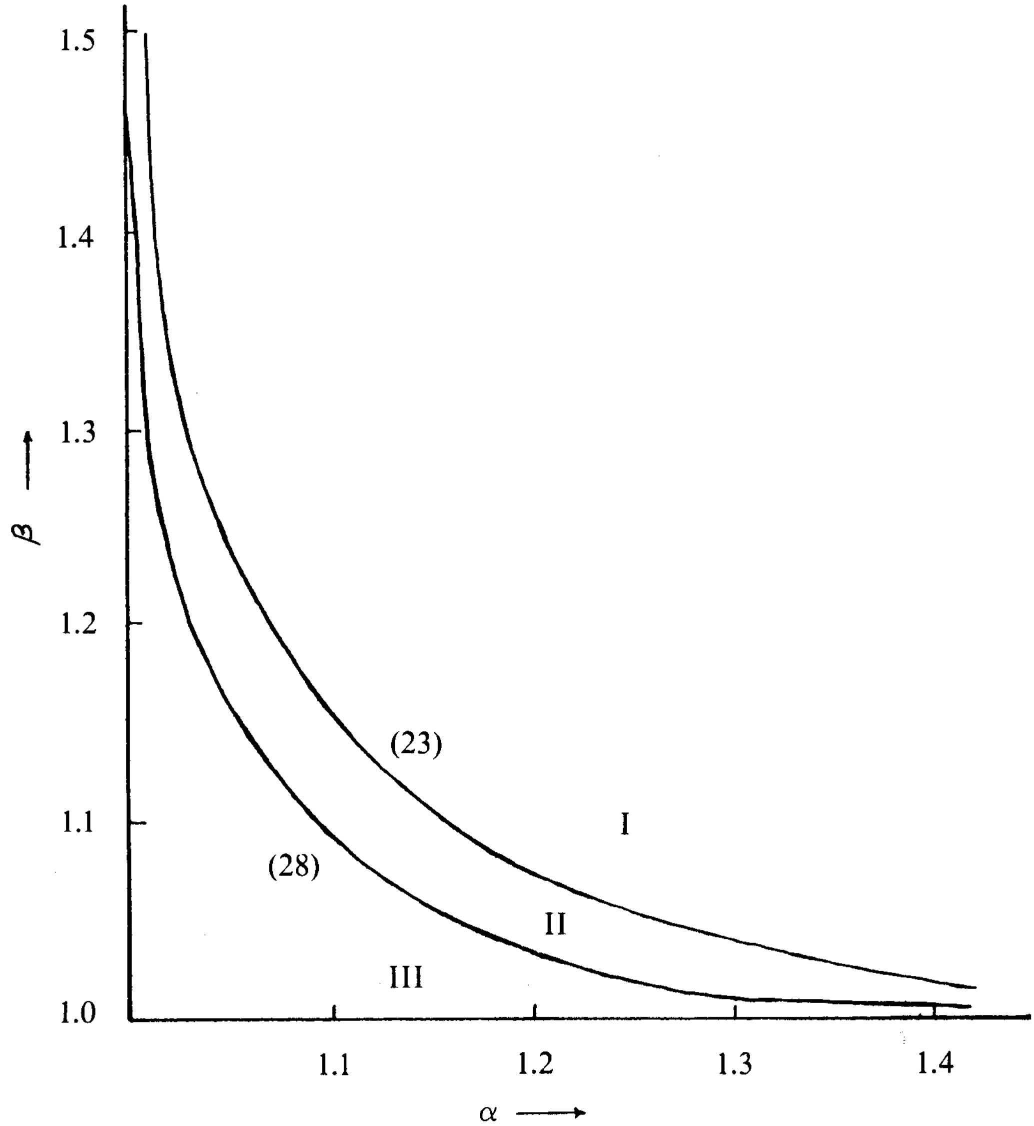

Fig. 2 Classification of dynamic behavior in the parameter space.

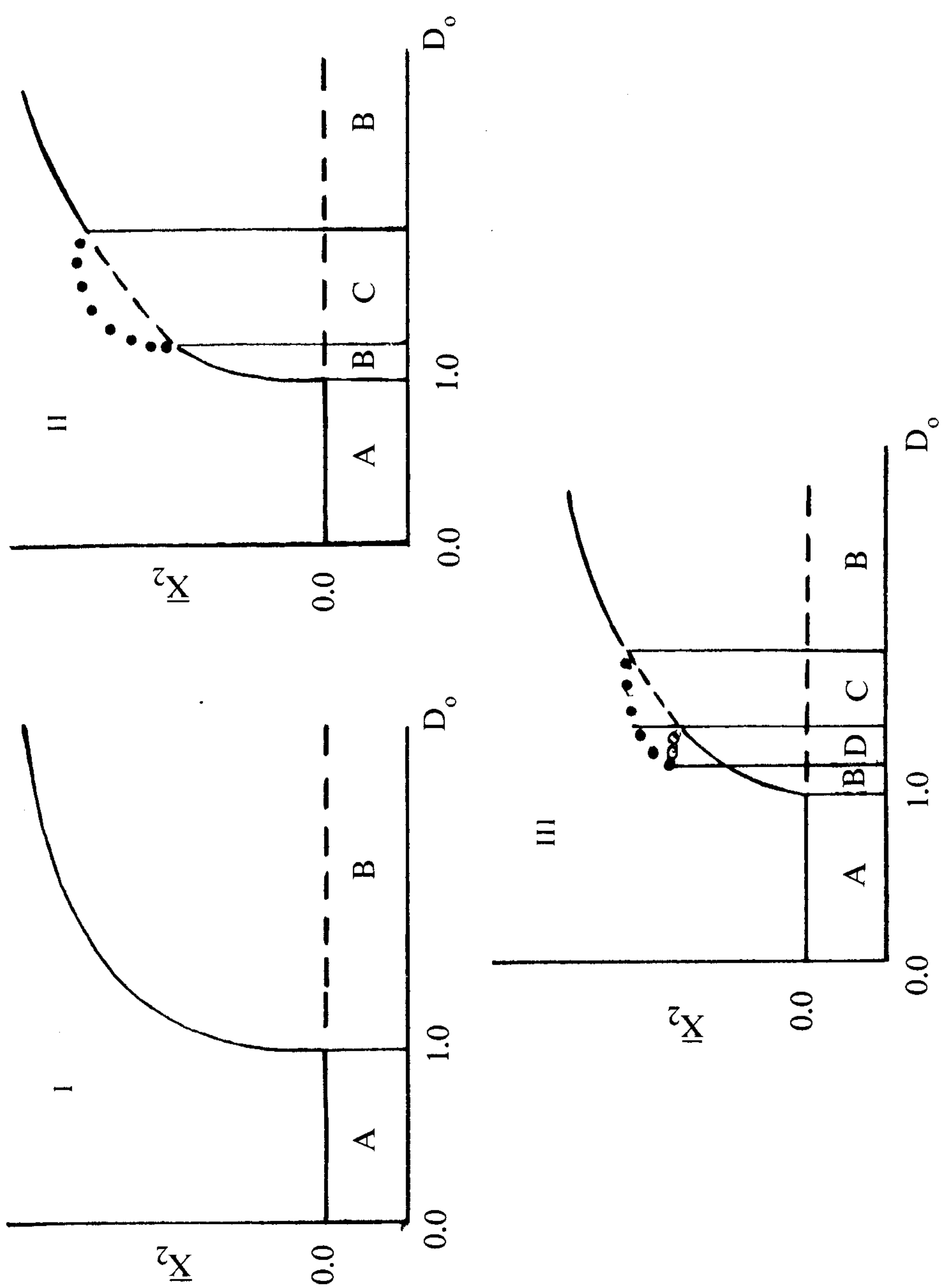

Fig. 3 Classification of dynamic behavior in $\bar{x}_2$ vs D_0 : —— stable steady state, --- unstable steady state, ... stable limit cycle, o o o unstable limit cycle.

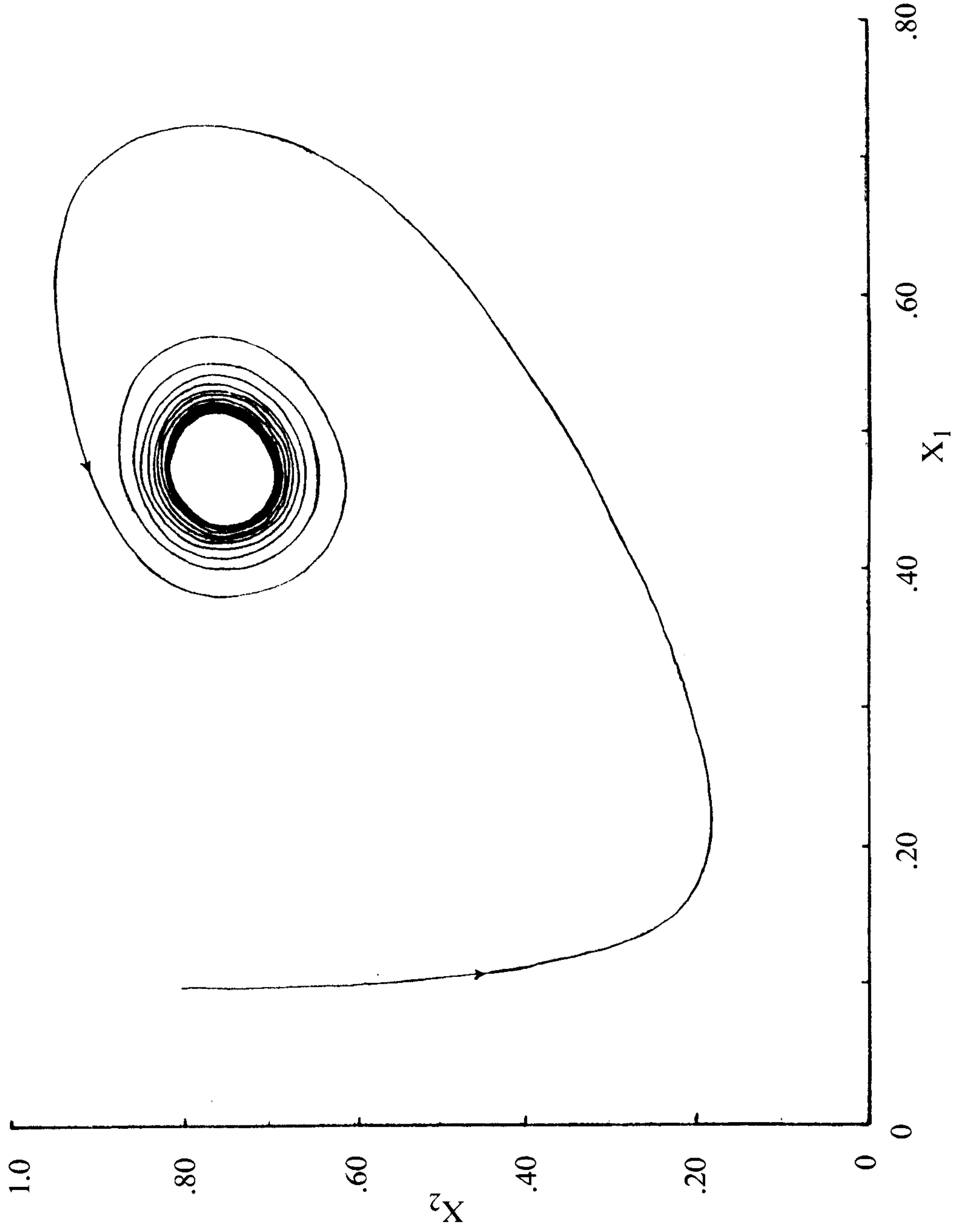

Fig. 4 Simulation of a type C phase–plane trajectory for α = 1.15, β = 1.10 and D_0 = 1.40.

These are equivalent to

$$(d\,\mu/dP)_{P=K_i x_2} < 0 \tag{18}$$

and

$$(d\,\sigma/dP)_{P=K_i x_2} = \sigma\, K_1/P < 0. \tag{19}$$

This means that, at the point of bifurcation, an increase in product concentration must decrease the specific growth rate and increase the production rate. Possible regions of bifurcation are indicated by the shaded portion in Fig.1

Now, onset of instability occurs when

$$\text{tr } J = 0 \text{ and } (\text{tr } J)' = 0. \tag{20}$$

We note that the denominator of tr J is always positive for $0<\bar{x}_2<1$ and tr J $= -1$ at $\bar{x}_2 = 0$ while tr J $\to -\infty$ when $\bar{x}_2 \to 1^-$.

Using (7) and (8), condition (20) is satisfied when

$$g(\bar{x}_2) = 0 \text{ and } g'(\bar{x}_2) = 0. \tag{21}$$

where $g(\bar{x}_2)$ is the numerator of tr J and

$$g(\bar{x}_2) \equiv 2\bar{x}_2^3 - (3+\phi)\bar{x}_2 + 2\phi\bar{x}_2 - \eta \tag{22}$$

where $\phi \equiv \alpha + \beta$, $\eta \equiv \alpha\beta$.

Then, condition (21) can be expressed as

$$\Omega(\alpha,\beta) \equiv 3(1+\eta-\phi)^{1/3} + \phi - 1 = 0 \tag{23}$$

For dynamic instability tr $J>0$ and, from Eq. (23), this requires that

$$1 > \phi + 3(1+\eta-\phi).^{1/3} \tag{24}$$

Let P_1 and P_2 be the two positive real roots of tr J $= 0$, the third root of the cubic equation being negative. Corresponding to P_1 and P_2 we have two critical values $D_{0,1}$ and $D_{0,2}$ given by

$$D_{0,1} = \frac{\alpha - P_1}{\alpha(1-P_1)} \qquad i = 1, 2. \tag{25}$$

Thus, bifurcation to periodic solutions occurs at two points for this system. As D_0 increases beyond the value of unity a stable nontrivial steady state appears until the lower critical value $D_{0,1}$, corresponding to the bifurcation point P_1, is reached where tr J $= 0$. At this point bifurcation to periodic solutions occurs. As D_0 increases further, tr J becomes positive, causing an unstable nontrivial steady state, until the upper critical value $D_{0,2}$ is reached and tr J $= 0$ again.

Agrawal[1] derived the condition for the stability of limit cycles for the microbial flow reactor. Comparison of their model with ours, leads to the following expression for asymptotically orbitally stable periodic solutions,

$$\Gamma_1(\alpha,\ \beta) \equiv [1 - P_1 - (\alpha - 1)\Theta_1\ (1 + \Theta_1)]\ (9P_1/\Theta_1 - 1 - 8P_1/3)$$
$$- 9(\alpha - 1)\ \ P_1\Theta_1^2 < 0\ ,\qquad i = 1, 2, \tag{26}$$

and $$\Theta_1 = (\beta - P_1)/(\alpha - P_1). \tag{27}$$

CLASSIFICATION OF THE DYNAMIC BEHAVIOR

The two parameters α and β, therefore, determine the stability regions of bifurcating periodic solutions. Numerical results show that inequality (26), with $i = 2$, is always satisfied for the values of $a \geq 1$ and $\beta \geq 1$ for which (24) holds. This means that bifurcations occurring at the upper critical value $D_{0,2}$ are always stable. This is not the case, however, for $D_{0,1}$. Fig.2 shows three regions of different dynamic behavior in the parameter space delineated by the graphs of Eqs. (23) and

$$\Gamma_1\ (\alpha,\ \beta) = 0. \tag{28}$$

In region I, there is no bifurcation since here $\Omega(\alpha,\ \beta) > 0$. In region II, there are stable bifurcations and in region III, bifurcation are unstable at $D_{0,1}$ but stable at $D_{0,2}$.

Following the representation used by Uppal,[4] we show in Fig.3 plots of $\bar{x}_2$ vs D_0 for each of the three regions. There can be four different types of different phase – plane trajectories corresponding to different ranges of D_0 values, and they are labelled A through D in Table 1.

In particular, three types of phase – plane are possible in region II, namely A, B and C. Type C phase – plane has an unstable washout steady state, which turns out to be a saddle point, and an unstable nontrivial steady state which is surrounded by a stable limit cycle. For this type of phase – plane, D_0 lies between $D_{0.1}$ and $D_{0.2}$, in which range tr $J > 0$.

Four types of phase – plane are possible in region III, A through D. We have unstable bifurcation at $D_{0,1}$ and a stable bifurcation at $D_{0,2}$.

In Fig.3, the solid line represents stable steady states while unstable steady states are represented by the dashed line. Stable limit cycles are denoted by dots and the distance between the dots and the dashed line approximately represents the average amplitude of the limit cycle which surrounds the unstable stedy state. Finally, Fig.4 shows a phase – plane trajectory showing the stable limit cycle which bifurcates from the unstable steady state. This is a type C phase – plane with D_0 lying between $D_{0.1}$ and $D_{0.2}$.

CONCLUSIONS

This note follows closely the work of Agrawal.[1] They employed the Monod's model and the two parameter hump function for the specific growth rate. We, on the other hand, used a product inhibition model and a decreasing specific growth function which may be considered as a combination of the Monod's model and that proposed by Yano and Koga. We note that with suitable changes of parameters, our product inhibition model (5) through (8) reduces to Agrawal's model of substrate inhibition model in their dimensionless form. We find that the necessary conditions for bifurcation are that the specific growth rate must decrease and the specific production rate must increase with the increase of product concentration. Moreover, bifurcations can not occur at the washout steady state and limit cycles, bifurcating only from the nontrivial steady state, exist for suitable values of the dilution rate. Thus, we have completely classified the possible dynamic behavior in the parameter space for the two parameters product inhibition model consisting of equations (1) through (4).

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บทคัดย่อ

ตัวแบบทางคณิตศาสตร์ของขบวนการหมักแบบต่อเนื่อง ซึ่งมีลักษณะการกีดกั้นโดยผลิตผล ซึ่งประกอบด้วยระบบของสมการเชิงอนุพันธ์ไม่เชิงเส้นสองสมการ ได้มีการนำมาพิจารณาพร้อมกับฟังก์ชันของอัตราการเจริญเติบโตสัมพัทธ์ ซึ่งได้รับการเปลี่ยนแปลงแก้ไข เพื่อได้มาซึ่งสมการขอบเขตที่จะแบ่งสเปซของพารามิเตอร์ออกเป็นส่วน ๆ โดยที่คำตอบของตัวแบบจะมีพฤติกรรมแตกต่างกันไปในแต่ละบริเวณนี้