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Analysis of a chemostat model with variable yield coefficient

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We investigate a chemostat model in which the growth rate is given by a Monod expression with a variable yield coefficient. This model has been investigated by previous researchers using numerical integration. We combine analytical results with path-following methods. The conditions for washout to occur are found. When washout does not occur we establish the conditions under which the reactor performance is maximised at either a finite or infinite residence time. We also determine the parameter region in which oscillations may be generated in the reactor, which was the primary feature of interest to earlier workers on this problem.

KEY WORDS: bioreactors, Non-linear dynamics, reaction engineering

AMS Subject classification: 34Cxx, 92C45, 92E20

1. Introduction

The past four decades have seen extensive research aimed at improving product yields in chemical reactors. Many studies, both experimental and theoretical, have shown that periodic forcing is an appropriate engineering tool to improve the conversion or selectivity of a desired product [1,2]. However, the additional complications and costs associated with implementing external periodic operation have limited the industrial uptake of this technique [1,2].

The possibility of combining the advantages of periodic operation with the benefits of using two reactors arranged in series through the use of 'natural oscillations' has been investigated by several authors [3–6]. By 'natural oscillations'

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it is meant that the process parameters are chosen so that a *steady input* of reactants into the first reactor generates *self-sustained oscillations* in its output. This output then forces the second reactor. The attraction of this method is that no external energy is required to generate the oscillations. Improvements in reactor performance are therefore achieved without the additional costs associated with external periodic forcing. Consequently, this approach harnesses the advantages of periodic forcing without the expense of its implementation.

We consider the case of a *single* reactor. The reason for this is that the two-reactor scenario considered by [3,6] does not include refluxing. Consequently the conditions under which natural oscillations are generated in the first reactor are determined purely by the dynamics of that reactor. As the point is to generate natural oscillations in the first reactor to force the second reactor it seems appropriate to determine the conditions under which such oscillations occur in the first reactor, before investigating the two-reactor system. We also believe that it does not make sense to maximise the output from a two-reactor system unless the maximum output from the single reactor system is available as a benchmark. Balakrishnan & Yang [7] examined the single reactor problem by directly integrating the model equations for a limited range of parameter values. In contrast we analyse the model by applying bifurcation theory and path-following methods.

2. Model equations

We investigate a microbial system in which cell mass (X) grows through consumption of a substrate species (S). The specific growth rate, equation (3), is given by a Monod expression with variable yield coefficient, equation (4), but without product and substrate inhibition. The problem is to maximise the cell mass concentration leaving the reactor as a function of the residence time. This microbial system was investigated earlier by [3,6,7]. The model used in this paper is a very simplisitic bioreactor model; more detailed models are available in the literature. Nevertheless, we have used it because of the attention it has drawn in the bioreactor engineering community.

The dimensional and dimensionless forms of our model are stated in sections 2.1 & 2.2 respectively.

2.1. Dimensional model

Following [7], the governing equations of our system are given by

$$V\frac{\mathrm{d}S}{\mathrm{d}t} = F(S_0 - S) - VX\frac{\mu(S)}{Y(S)} \tag{1}$$

$$V\frac{\mathrm{d}X}{\mathrm{d}t} = F(X_0 - X) + VX\mu(S) \tag{2}$$

Specific growth rate equation

$$\mu(S) = \frac{\mu_m S}{K_s + S} \tag{3}$$

Yield Coefficient

$$Y(S) = \alpha + \beta S, \quad (\alpha, \beta > 0) \tag{4}$$

The terms that appear in equations (1–4) are defined in the nomenclature.

2.2. Dimensionless equations

By introducing dimensionless variables for the substrate concentrations ($S^* = S/K_s$), the cell mass concentrations ($X^* = X/(\alpha K_s)$) and time ($t^* = \mu_m t$) the system of differential equations (1) and (2) can be written in the dimensionless form

$$\frac{dS^*}{dt^*} = \frac{1}{\tau^*}\left(S_0^* - S^*\right) - \frac{S^* X^*}{(1 + \beta^* S^*)(1 + S^*)}, \tag{5}$$

$$\frac{dX^*}{dt^*} = \frac{1}{\tau^*}\left(X_0^* - X^*\right) + \frac{S^* X^*}{1 + S^*}. \tag{6}$$

The dimensionless model contains four parameters S_0^*, X_0^*, β, τ^*. We consider the case of a sterile feed ($X_0^* = 0$) and take the residence time (τ^*) as the primary bifurcation parameter. The substrate concentration in the feed (S_0^*) and the dimensionless yield coefficient (β^*) are the secondary bifurcation parameters. The value for β^* is determined by the choice of microbial system and is therefore not a 'tunable' parameter.

A feature of our dimensionless scheme is that there is a one-to-one relationship between our dimensionless variables and their dimensional counterparts. Hence we write often, for example, 'the residence time', rather than 'the dimensionless residence time'.

2.3. Numerics

The path-following software Auto 97 [8] was used to obtain the steady-state diagrams. In these the standard representation is used; solid lines are stable steady states; dotted lines are unstable steady states; squares are Hopf bifurcation points; open circles are unstable periodic orbits and filled-in circles are stable periodic solutions. We investigate the reactor performance (X^*) as a function of the residence time (τ^*). For a periodic orbit the norm that is used is the integral over the period of the solution.

3. Results

3.1. Analytical results: steady-state solutions and their stability

3.1.1. Steady-state solutions

The model (5) & (6) has two steady-state solutions. These represent washout and no washout in the reactor and are given by

Washout

$$\left(S^*, X^*\right) = \left(S_0^*, 0\right), \tag{7}$$

No washout

$$\left(S^*, X^*\right) = \left(\frac{1}{\tau^* - 1}, \frac{S_0^*\tau^* - \left(1 + S_0^*\right)}{\tau^* - 1} \cdot \frac{\tau^* + (\beta^* - 1)}{\tau^* - 1}\right). \tag{8}$$

The substrate component of (8) is positive only if $\tau^* > 1$. Given that $\tau^* > 1$ the cell mass component of (8) is non-negative only if $\tau^* \geqslant 1 + \frac{1}{S_0^*}$. Thus the no washout solution is only physically meaningful if

$$\tau^* \geqslant 1 + \frac{1}{S_0^*}.$$

It is instructive to investigate how the steady-state performance of the reactor, that is to say the value of the cell mass concentration on the non-washout state, varies with the residence time. In particular, we want to determine whether there is a residence time at which the cell-mass concentration is maximised.

Calculation shows that

$$\frac{\mathrm{d}X^*}{\mathrm{d}\tau^*} = 0 \Leftrightarrow \tau^*_{\max} = 1 + \frac{2\beta^*}{\beta^* S_0^* - 1}, \tag{9}$$

subject to the restriction that $\tau^*_{\max} \neq 1$. It follows that if $\beta^* S_0^* > 1$ the steady-state diagram of system performance (X^*) against residence time (τ^*) has a local maximum at the point

$$\left(\tau^*, X^*\right) = \left(\tau^*_{\max}, \frac{\left(1 + \beta^* S_0^*\right)^2}{4\beta^*}\right). \tag{10}$$

Conversely, if $\beta^* S_0^* < 1$ then this implies that $\tau^*_{\max} < 1$ and the corresponding value of X^* is non-physical. In this case, the steady-state performance is maximised at an infinite residence time

$$\lim_{\tau^* \to \infty} X^* = S_0^*.$$

3.1.2. Stability of the washout state

The Jacobian matrix for the washout state is

$$J = \begin{pmatrix} -\dfrac{1}{\tau^*} & \dfrac{-S_0^*}{\left(1+\beta^* S_0^*\right)\left(1+S_0^*\right)} \\ 0 & -\dfrac{1}{\tau^*} + \dfrac{S_0^*}{1+S_0^*} \end{pmatrix}. \tag{11}$$

This has eigenvalues

$$\lambda_1 = \frac{-1}{\tau^*}, \qquad \lambda_2 = \frac{S_0^*}{1+S_0^*} - \frac{1}{\tau^*}.$$

The washout state is therefore stable if

$$\tau^* < 1 + \frac{1}{S_0^*}. \tag{12}$$

3.1.3. Stability of the no washout state

The Jacobian matrix for the no washout state is

$$J = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & 0 \end{pmatrix}, \tag{13}$$

where

$$J_{11} = \frac{-S_0^* t^{*^3} + 3S_0^* t^{*^2} - \left[3S_0^* + 1 + \beta^*\left(1 - S_0^*\right)\right] t^* - \left(\beta^* - 1\right)\left(1 + S_0^*\right)}{t_1^{*^2}\left[t_1^* + \left(\beta^* - 1\right)\right]}, \tag{14}$$

$$J_{12} = \frac{-\left(\tau^* - 1\right)}{\tau^*\left(\tau^* - 1 + \beta^*\right)}, \tag{15}$$

$$J_{13} = \frac{\left(S_0^*\tau^* - 1 - S_0^*\right)\left(\tau^* + \beta^* - 1\right)}{\tau^*}. \tag{16}$$

The Jacobian matrix (13) has a zero eigenvalue when $J_{12}J_{21} = 0$. This requires τ_1^* to take value $1 - \beta^*$, 1 or $1 + \frac{1}{S_0^*}$. In view of the discussion in section 3.1.1. only the condition $\tau_1^* = 1 + \frac{1}{S_0^*}$ is relevant.

The conditions for a double-zero eigenvalue are $J_{12}J_{21} = 0$ and $J_{11} = 0$ [9]. These conditions are satisfied when $\tau_1^* = 1 + \frac{1}{S_0^*}$ *and* either $S_0^* = -1$ or $S_0^* = \frac{-1}{\beta^*}$. The negative concentration of the substrate concentration in the feed immediately implies that a double-zero eigenvalue can not occur.

We know that when $\beta^* S_0^* > 1$ there is a value of the residence time that maximises the reactor performance. From the Jacobian matrix (13) this point is stable if

$$J_{11} < 0,$$
$$-J_{12} \cdot J_{21} > 0.$$

The appropriate values of τ^*, S^* and X^* ($\tau^*_{\max}$, $S^*_{\max}$ and $X^*_{\max}$) are found by combining equations (8–10). After some algebraic manipulation we obtain

$$J_{11} = -\frac{2\left(S_0^*\beta^* + 1\right)\beta^*}{\left(S_0^*\beta^* - 1 + 2\beta^*\right)^2},$$
$$-J_{12}\cdot J_{21} = \frac{2\left(S_0^*\beta - 1\right)\beta\left(S_0^*\beta^* + 1\right)}{\left(S_0^*\beta^* - 1 + 2\beta^*\right)^3}.$$

As $X^*_{\max}$ only exists if $S_0^*\beta^* - 1 > 0$ we conclude that the point $(S^*_{\max}, X^*_{\max})$ is *always* stable and is therefore of practical importance.

3.1.4. Hopf bifurcations on the no washout state

The condition for a Hopf bifurcation is $J_{11} = 0$ with $J_{12}J_{21} < 0$ [9]. The latter implies that $\tau_1^* > 1 + \frac{1}{S_0^*}$. The values of the residence time at which Hopf bifurcations occur correspond to the roots of

$$\mathcal{H}\left(\tau^*\right) = -S_0^*\tau^{*^3} + 3S_0^*\tau^{*^2} - \left[3S_0^* + 1 + \beta^*\left(1 - S_0^*\right)\right]\tau^* - \left(\beta^* - 1\right)\left(1 + S_0^*\right) = 0 \tag{17}$$

subject to the constraint $\tau^* > 1 + \frac{1}{S_0^*}$. It is possible to show that if $\beta^* > 1$ then equation (17) always possess at least one root with $\tau^* < 0$.

A degenerate Hopf bifurcation at which two Hopf points annhilate each other in an unfolding diagram (a $H2_1$ degeneracy) occurs when the following conditions are satisfied [9]

$$\mathcal{H} = 0, \tag{18}$$
$$\frac{d\mathcal{H}}{d\tau^*} = 0. \tag{19}$$

When applied to equation (17) these conditions give the following system of equations

$$S_0^* = \frac{1 + \beta^*}{-3\tau^{*^2} + 6\tau^* - 3 + \beta^*}, \tag{20}$$
$$0 = \left(1 + \beta^*\right)\tau^{*^3} - 3\tau^{*^2} - 3\left(\beta^* - 1\right)\tau^* - \left(\beta^* - 1\right)^2 = \mathcal{J}\left(\tau^*\right). \tag{21}$$

Note that the function $\mathcal{J}$ has the following properties

$$\mathcal{J}(1) = -\left(\beta^*\right)^2 < 0, \tag{22}$$
$$\mathcal{J}\left(\tau_1^* \to \infty\right) > 0. \tag{23}$$

Furthermore, assuming that $\beta^* > 0$, $\mathcal{J}$ has a local maximum when $\tau^* = \frac{1-\beta^*}{1+\beta^*} < 1$ with

$$\mathcal{J}\left(\frac{1-\beta^*}{1+\beta^*}\right) = -\frac{\beta^{*^2}(1-\beta^*)^2}{(1+\beta^*)^2} \leqslant 0$$

and a local minimum when $\tau^* = 1$. Thus we conclude that for $\beta^* > 0$ there is a unique $H2_1$ degeneracy with $1 < \tau^* < \infty$.

For the parameter values used in [3,6,7] (corresponding to $\beta^* = 5.25$) the solution of equations (20) & (21) is

$$\left(S_0^*, \tau^*\right) = (3.9097, 2.103)\,. \tag{24}$$

Natural oscillations are impossible for $\beta^* = 5.25$ if the substrate concentration is sufficiently small ($S_0^* < 3.9097$ or $S_0 < 6.84203\,\mathrm{gl}^{-1}$). The work reported in [3, 6,7] used $S_0 \geq 10\,\mathrm{g\,l}^{-1}$. Thus conditions under which natural oscillations are not generated were not reported.

3.2. *Numerical results: steady-state diagram*

Figure 1 shows three steady-state diagrams when $\beta^* = 5.25$, which is the value used in [3,6,7]. The first steady-state diagram contains two Hopf points. In the second and third steady-state diagrams there are no Hopf points as the inflowing substrate concentration is below that corresponding to the $H2_1$ degeneracy. In (a and b) $\beta^* S_0^* > 1$ so that the steady-state value of the reactor-performance (X_1^*) is maximised at a finite value of the residence time. In (c) $\beta^* S_0^* < 1$, so that the system performance increases monotonically with the residence time. For this particular system $X_{\max}^* = \frac{1}{21} \approx 0.0476$. Only the first of these steady-state diagrams is presented in [3,6,7].

The two Hopf bifurcation points in figure 1(a) are unfolded with the substrate concentration in the feed in figure 2. This shows that as the substrate concentration is decreased the two Hopf points annihilate each other at a $H2_1$ degeneracy for the values stated by equation (24).

Figure 3 shows the $H2_1$ locus in the inflow substrate concentration-yield coefficient plane. For a fixed value of the latter the steady-state diagram has *no* Hopf points if the value of the inflowing substrate concentration is *below* the $H2_1$ locus and *two* Hopf points if it is above. This figure also contains the line $S_0^*\beta^* = 1$. The reactor performance has a local maximum at a finite value of the residence time if $S_0^*\beta^* > 1$. If $S_0^*\beta^* < 1$ then the reactor performance is optimised at infinite residence time. It is not difficult to show that these lines do not intersect. Thus the three steady-state diagrams illustrated in figure 1 cover the range of generic behaviour exhibited by this system.

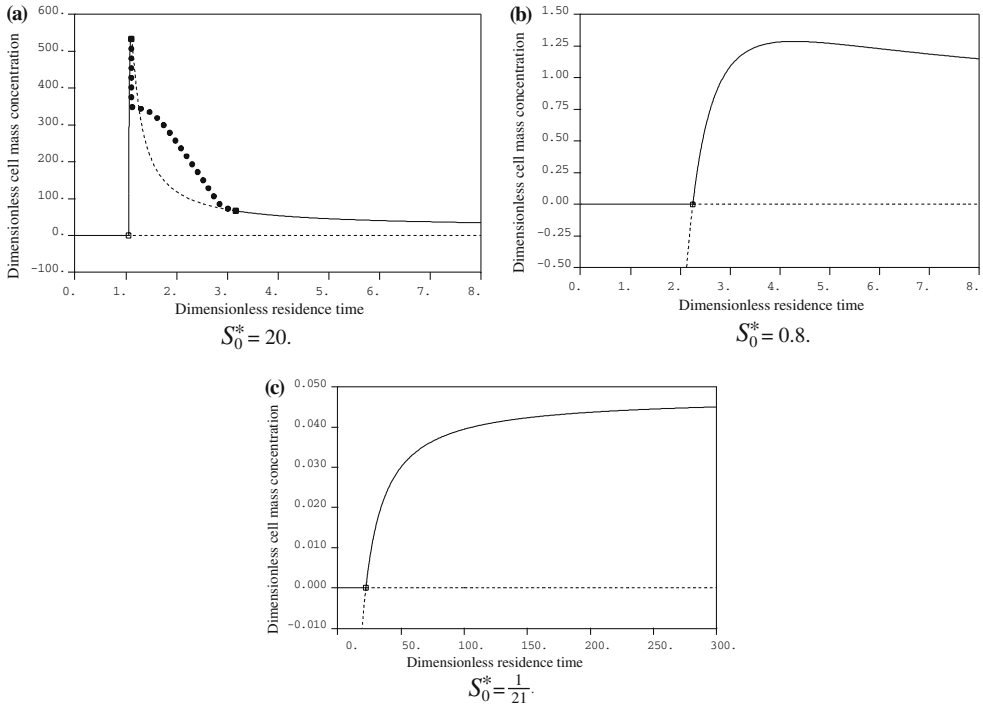

Figure 1. Steady-diagrams showing the variation of reactor performance (X_1^*) with residence time (τ_1^*). Parameter value: $\beta^* = 5.25$.

4. Conclusion

We have analysed a simple model for microbial growth in a flow reactor that has previously been investigated by numerical integration for two bioreactors in series [3,6] and for a single reactor [7]. The focus in earlier work was in using natural oscillations generated in the first reactor to force a second reactor.

For a given value of the yield coefficient (β^*) we have shown that natural oscillations only occur if the substrate concentration in the feed (S_0^*) is sufficiently high. If this condition holds then natural oscillations are generated, the phenomena of primary interest in [3,6,7], when $H_1 < \tau^* < H_2$, where H_1 and H_2 are appropriate roots of equation (17).

An important result of this paper is that if $\beta^* S_0^* > 1$ there is a value of the residence time, $\tau_{\max}^*$ given by equation (9), at which the steady-state performance of the reactor is maximised, $X_{\max}^*$ given by equation (10). If $\beta^* S_0^* < 1$ then the steady-state performance of the reactor is maximised at an infinite residence time, with $X_{\max}^* = S_0^*$.

Consider a system of two bioreactors in which the residence time in the two reactors are varied whilst keeping the total residence time fixed. The maximal

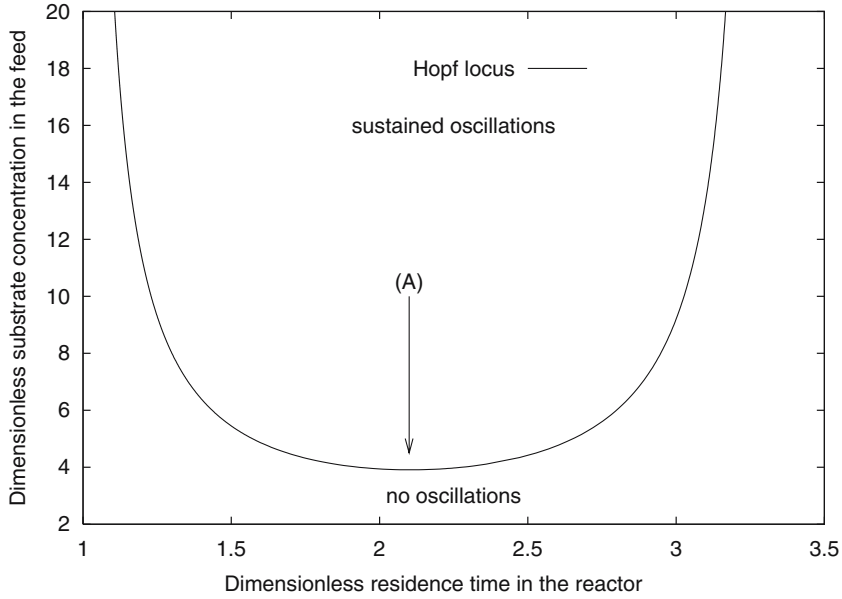

Figure 2. Hopf point unfolding curve showing the destruction of the two Hopf points at a $H2_1$ degeneracy (A). Parameter value: $\beta^* = 5.25$.

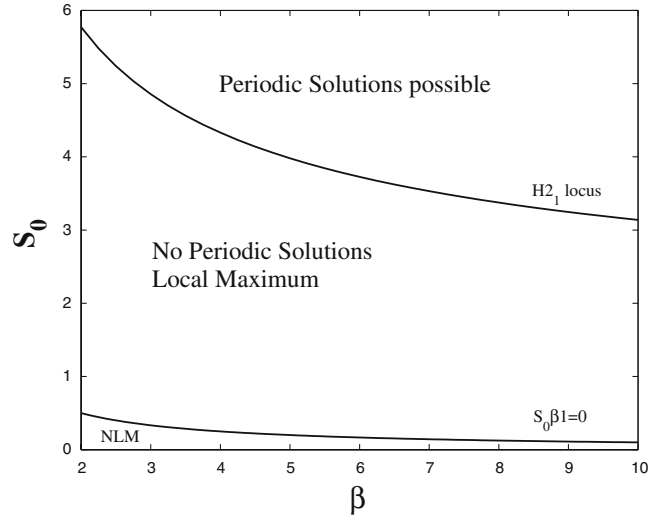

Figure 3. Bifurcation diagram showing the $H2_1$ locus and the transition from a steady-state diagram having a local maximum to not having a local maximum (NLM). (Compare figures 1 (a and b) with figure 1 (c). Parameter value: $\beta^* = 5.25$.

performance of this system should be compared against that of the one-reactor system to evaluate the relative increase in performance from using two reactors. Such a comparison was not made in [3,6].

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A Nomenclature

F	Flowrate	$(\mathrm{l\,hr^{-1}})$
K_s	Monod constant	$(\mathrm{g\,l^{-1}})$
S	Substrate concentration	$(\mathrm{g\,l^{-1}})$
S^*	Dimensionless substrate concentration $S_i^* = \frac{S_i}{K_s}$	(—)
S	Substrate concentration in the feed	$(\mathrm{g\,l^{-1}})$
S_0^*	Dimensionless substrate concentration in the feed $S_0^* = \frac{S_0}{K_s}$	(—)
V	Reactor volume	(l)
X	Cell mass concentration	$(\mathrm{g\,l^{-1}})$
X^*	Dimensionless cell mass concentration $X_i^* = \frac{X_i}{\alpha K_s}$	(—)
X_0	Cell mass concentration in the feed	$(\mathrm{g\,l^{-1}})$
X_0^*	Dimensionless cell mass concentration in the feed $X_0^* = \frac{X_0}{\alpha K_s}$	(—)
$Y\,(S_i)$	Cell mass yield coefficient	(—)
t	Time	(h)
t^*	Dimensionless time $t^* = \mu_m t$	(—)
α	Constant in yield coefficient	(—)
β	Constant in yield coefficient	$(\mathrm{l\,g^{-1}})$
β^*	Dimensionless yield coefficient $\beta^* = \frac{\beta K_s}{\alpha}$	(—)
$\mu\,(S)$	Specific growth rate	$(\mathrm{h^{-1}})$
μ_m	Maximum specific growth rate	$(\mathrm{h^{-1}})$
τ	Residence time $\tau_i = \frac{V_i}{F}$	(h)
τ^*	Dimensionless residence time $\tau_i^* = \mu_m \cdot \frac{V_i}{F}$	(—)

Parameter values (from Yang and Su 1993, Yang and Balakrishnan, 2002): $K_s = 1.75\,\mathrm{g\,l^{-1}}$, $\alpha = 0.01$, $\beta = 0.031\,\mathrm{g^{-1}}$, $\mu_m = 0.3\,\mathrm{h^{-1}}$. These give $\beta^* = 5.25$.

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