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ORIGINAL PAPER

Global analysis of continuous flow bioreactor and membrane reactor models with death and maintenance

Tonghua Zhang

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Abstract The aim of the paper is to investigate the global dynamics of mathematical models for a continuous flow bioreactor and a membrane reactor. It assumes that the models include terms representing death of the microorganism and maintenance energy, respectively. By carrying out a qualitative analysis of the models, we give the classification of the equilibria and show that an unstable limit cycle can exist when the non-washout equilibrium is a focus.

Keywords Dynamics · Qualitative analysis · Continuous flow bioreactor model · Membrane reactor model · Limit cycle · Equilibrium

1 Introduction

Industrial effluent and household sewage are complex mixtures of many substrates and microorganisms. The purpose of wastewater treatment is to remove pollutants what can harm the aquatic environment. Although continuous flow reactors have commonly been used in the treatment of industrial wastewater, membrane reactors are especially designed for domestic wastewater treatment [10]. Let $S(t)$ be the concentration of substrate within the bioreactor, $X(t)$ be the concentration of microorganism at time t, respectively. Monod developed a simply mathematical model [9], rewriting which into the dimensionless form it is given as follows.

$$\begin{aligned} \frac{dS}{dt} &= \frac{S_0 - S}{\tau} - Xg(S) \\ \frac{dX}{dt} &= -\frac{X}{\tau} + Xg(S) \end{aligned} \tag{1.1}$$

T. Zhang (✉)
Mathematics, H38, FEIS, Swinburne University of Technology, Hawthorn, VIC 3122, Australia
e-mail: tonghuazhang@swin.edu.au

where the Monod growth rate is given by

$$g(S) = \frac{S}{1+S} \tag{1.2}$$

It is now also known as the "chemostat model", which along with the extended models has been intensively studied, to name but a few [1–6,8–17,21]. Fan and Wolkowicz [1], Ruan [14], Wolkowicz and Xia [17] and Yuan and Zhang [20] investigated models with time delay; Huang et al. [2–4,21] investigated a model with quadratic yield and toxin; Imhofa and Walcherb [5] investigated a stochastic model and Nelson et al. [10–12] investigated models with different kinetics. By Monod's study, the nontrivial steady-state of model (1.1) can only exist when the residence time, τ is sufficiently large. Using phase-plane approach [6], Koga and Humphrey investigated the global dynamics of model (1.1) and they found the sustained oscillation could not happen. When τ is not large, model matches well with the experimental data. However, there is a noticeable discrepancy when τ is very large [10]. To overcome this, a extra term, $-k_d X$ was introduced to the model, which had been studied by McCarty [8]. However, the stability of the non-washout equilibrium has not been studied. Later on, another term of $-m_s X$ was introduced to the model, which is used to represent the maintenance energy when τ is large. A different type of growth model, which is now known as the Tessier growth model was used by Tessier when he investigated a model with maintenance [16]. Pirt [13] investigated the case of Monod growth model, and Koga and Humphrey [6] studied the case of $m_s > 0$ and $k_d = 0$. A similar mathematical model can also developed for the recycle reactor. According to the openly published literature, no results on the stability analysis of a mathematical model including either death of microorganisms or maintenance for flow and recycle reactors has been published before the work of Nelson et al. [10]. In this work, they considered the model governed by

$$\begin{aligned} V\tfrac{dS}{dt} &= F(S_0 - S) - \tfrac{\mu(S)}{\alpha} VX - Vm_s X, \\ V\tfrac{dS}{dt} &= \beta F(X_0 - X) + \gamma RF(C-1)X + VX\mu(S) - Vk_d X \end{aligned} \tag{1.3}$$

where the growth rate, $g(S)$ and the residence time are given respectively by

$$g(S) = \frac{\mu_m S}{K_s + S},$$
$$\tau = \frac{V}{F}$$

where, for specific process, K_s, k_d, m_s, α and μ_{max} are fixed, S_0, X_0 and τ are parameters which can be varied and β and γ are parameters defined the reactor model with $\beta = \gamma = 1$ gives a continuous flow reactor and $\beta = \gamma = 0$ gives an idealised membrane reactor in which all the microorganisms are constrained to remain in the reactor vessel.

However, in that paper, the global dynamics of model (1.3) has not been investigated, such as the existence, non-existence of limit cycle, the uniqueness if it exists. Our intention here is to give a globally qualitative analysis for model (1.3) from the mathematical point of view. The rest of the paper is organised as follows. In Sect. 2, we shall convert the model interested into a dimensionless version and specify the case we study. In the first part of Sect. 3, by using the results from [10] or direct analysis, we give the classification of the washout equilibrium, E_1; and then give the condition of existing a non-washout equilibrium, E_2 and its type. In the second part of Sect. 3, we discuss when the limit cycle can not exist and when we can have a limit cycle; if it exists, the uniqueness and stability of it shall also be proven. We then conclude the paper in Sect. 4.

2 Mathematical model

By using the transformations introduced in [10], the above dimensional model (1.3) can be converted into the following dimensionless form, for more details we refer readers to reference [10]. For notation simplicity, we still use the original symbols in the new model.

$$\begin{aligned} \tfrac{dS}{dt} &= \tfrac{1}{\tau}(S_0 - S) - \tfrac{SX}{1+S} - m_s X, \\ \tfrac{dX}{dt} &= \beta \tfrac{1}{\tau}(X_0 - X) + \gamma \tfrac{R}{\tau} X + \tfrac{SX}{1+S} - k_d X \end{aligned} \tag{2.1}$$

If assume that $X_0 = 0$, namely there is no microorganism in the influent, then from the analysis of [10], the dynamics of a reactor model with idealised recycle is equivalent to the idealised membrane reactor, and that of a reactor model with non-idealised recycle is equivalent to a non-idealised membrane reactor model. In other word, the case of $\beta = \gamma = R = 1$ is equivalent to the case of $\beta = \gamma = 0$ and the case of $0 < \beta < 1, \gamma = 0$ is equivalent to that of $\beta = \gamma = 1, 1 > R > 0$. Therefore, in this study we focus on the investigation of a flow reactor with recycle

$$\beta = \gamma = 1, 0 \le R \le 1$$

and $X_0 = 0$, $S_0 \neq 0$, and where $R = 0, 0 < R < 1$ and $R = 1$ correspond models of a flow reactor without recycle, a flow reactor with non-idealized recycle and a flow reactor with idealized recycle, respectively.

3 Mathematical analysis

3.1 Qualitative analysis of the equilibria

It is easy to see that system (2.1) always has a washout equilibrium $E_1(S_0, 0)$ for all three cases. In what follows, we shall investigate the type and stability of E_1 for each of these cases separately. Notice the Jacobian of model (2.1) at E_1 is given by

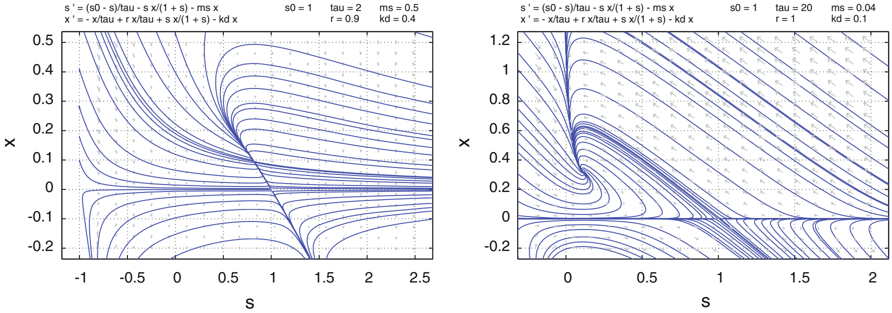

Fig. 1 Equilibria

$$J(S_0, 0) = \begin{vmatrix} -\frac{1}{\tau} & -\frac{S_0}{1+S_0} - m_s \\ 0 & -\frac{1}{\tau} + \frac{R}{\tau} + \frac{S_0}{1+S_0} - k_d \end{vmatrix} \tag{3.1}$$

from which we have the eigenvalues

$$\lambda_1 = -\frac{1}{\tau} \tag{3.2}$$

$$\lambda_2 = -\frac{1}{\tau} + \frac{R}{\tau} + \frac{S_0}{1+S_0} - k_d \tag{3.3}$$

By straightforward analysis or using results from [10], we can easily conclude the following Theorem 3.1.

Theorem 3.1 *For the washout equilibrium point, E_1 of system (2.1) with $\beta = \gamma = 1$, we have*

(1) for the case of a flow reactor without recycle (or with non-idealised recycle), namely $R = 0 (or\, 0 < R < 1)$, it is a stable node when $k_d \geq \frac{S_0}{1+S_0}$ or $k_d < \frac{S_0}{1+S_0}$ and $\tau < \frac{(1-R)(1+S_0)}{S_0-(1+S_0)k_d}$; otherwise it is a saddle point;

(2) for the case of a flow reactor with idealised recycle, namely $R = 1$, it is a stable node when $k_d \geq \frac{S_0}{1+S_0}$, while it is a saddle point when $k_d < \frac{S_0}{1+S_0}$.

Please see Fig. 1, which is the case of E_1 to be a saddle point.

As system (2.1) has at most two equilibria: the washout equilibrium, E_1 and a non-washout equilibrium, $E_2(S^*, X^*)$ where

$$S^* = \frac{1 - R + k_d\tau}{R - 1 + (1 - k_d)\tau},\, X^* = \frac{S_0 - S^*}{1 - R + (k_d + m_s)\tau} \tag{3.4}$$

To have E_2 physically meaningful, namely both S^* and X^* should be positive, one of the following conditions should be satisfied.

(i) $k_d < \frac{S_0}{1+S_0}$ and $\tau \geq \frac{(1-R)(1+S_0)}{S_0-(1+S_0)k_d}$ for $0 \leq R < 1$;

(ii) $k_d < \frac{S_0}{1+S_0}$ for $R = 1$.

Then from Theorem 3.1, when E_2 is a positive equilibrium the washout equilibrium E_1 is a saddle point.

Theorem 3.2 *When having physical meaning, E_2 is always stable; furthermore if $-2 < \delta$ it is a focus and if $\delta \leq -2$ it is a node, where δ is defined by equation* (3.10).

Proof First the stability of E_2 can be obtained directly from reference [10] or straightforward analysis. Next we shall prove when it is a focus and when it is a node. To this end, let's rewrite model (2.1) as

$$\begin{aligned} \frac{dS}{dt} &= \frac{1}{\tau}(S_0 - S)(1+S) - SX - m_s X(1+S) \equiv P_2, \\ \frac{dX}{dt} &= -\frac{1}{\tau}X(1+S) + \frac{R}{\tau}X(1+S) + SX - k_d X(1+S) \equiv Q_2 \end{aligned} \tag{3.5}$$

From the theory of quadratic curves, there is a real number, λ such that

$$\lambda P_2 + Q_2 = R_1 R_2$$

where R_i is a real polynomial in S and X with degree of which is not higher than 1. It is easy to see that $\lambda = 0$ is a smart choice and then we have

$$R_1 = X, R_2 = \frac{R-1}{\tau} - k_d + \left(\frac{R-1}{\tau} - k_d + 1\right) S$$

Introduce transformation

$$\bar{S} = R_2 \text{ and } \bar{X} = X \tag{3.6}$$

and then model (3.5) becomes

$$\begin{aligned} \frac{d\bar{S}}{dt} &= \frac{R-1+(1-k_d)\tau}{\tau} \left[\frac{\bar{S}+1}{R-1+(1-k_d)\tau} \left(S_0 + 1 - \frac{\tau(\bar{S}+1)}{R-1+(1-k_d)\tau} \right) \right. \\ &\quad \left. + \left(1 - \frac{\tau(\bar{S}+1)}{R-1+(1-k_d)\tau}\right) \bar{X} - m_s \bar{X} \frac{\tau(\bar{S}+1)}{R-1+(1-k_d)\tau} \right], \\ \frac{d\bar{X}}{dt} &= \bar{X}\bar{S} \end{aligned} \tag{3.7}$$

Notice that the determinant of the transformation (3.6)

$$\begin{vmatrix} \frac{\partial R_2}{\partial S} & \frac{\partial R_2}{\partial X} \\ \frac{\partial X}{\partial S} & \frac{\partial X}{\partial X} \end{vmatrix} = \frac{R - 1 + (1-k_d)\tau}{\tau} > 0 \tag{3.8}$$

which implies that system (3.5) is topologically equivalent to (3.7). Now shift the non-washout equilibrium, E_2 to the origin and introduce the second transformation

$$s = \frac{1}{\mu}\bar{S}, x = \frac{1}{\nu}\bar{X}, t' = \frac{1}{\lambda}t,$$

with

$$\lambda = \sqrt{\frac{\tau}{S_0 - S^*}}$$
$$\mu = \frac{1}{\lambda}$$
$$\nu = \frac{S_0 - S^*}{1 - R + (k_d + m_s)\tau}$$

After dropping off the prime, $'$ of t' we end up with

$$\frac{ds}{dt} = -x + \delta s + ls^2 + msx \qquad \frac{dx}{dt} = s(1 + x) \tag{3.9}$$

which is a quadratic system of class (III) with $n = a = 0$ and $b = 1$ (see [18] for more details on the classification of quadratic systems) and here

$$\delta = -\sqrt{\frac{\tau}{S_0 - S^*}} \frac{(R - 1 + (1 - k_d)\tau)}{\tau} \times \left[\frac{S_0 - S^*}{1 - R + (k_d + m_s)\tau} + \frac{\tau}{(R - 1 + (1 - k_d)\tau)^2} \right], \tag{3.10}$$

$$l = -\frac{1}{R - 1 + (1 - k_d)\tau}, \tag{3.11}$$

$$m = -(1 + m_s)\sqrt{\frac{\tau}{S_0 - S^*}} \frac{S_0 - S^*}{1 - R + (k_d + m_s)\tau} \tag{3.12}$$

Notice that $\delta < 0$ when E_2 exists. We know the determinant of the Jacobian at the origin of system (3.9) has two negative real roots when $\delta \leq -2$, otherwise, it has a pair of complex roots with negative real parts, which implies the conclusion. The proof is completed. □

3.2 Uniqueness of limit cycle

From previous section, it is easy to see if system (2.1) has a limit cycle, it must surround E_2 only as E_1 is a saddle point. Notice the fact that there is no term of x^2 in the first equation of system (3.9). By Theorem 15.3 of reference [18], we have the following lemma.

Lemma 3.1 *If system* (3.9) *has a limit cycle surrounding the origin, then it must be unique.*

We can also prove the following theorem.

Lemma 3.2 *When* $\delta \leq m$ *system* (3.9) *has no limit cycle surrounding the origin.*

Proof From the second equation of system (3.9), we know that if the limit cycle surrounding the origin exists, then it must locate in the half-plane, $x > -1$. Therefore we do a transformation, $s = y(1+x)^l$, $x = x$, which leads to a new system

$$\frac{dy}{dx} = \frac{-x + (mx+\delta)(1+x)^l y}{(1+x)^{2l+1} y} \tag{3.13}$$

It is equivalent to, if we let $\bar{y} = -y + \int_0^x (mx+\delta)(1+x)^{-l-1} dx$ and drop off the overhead bar for the sake of notation simplicity,

$$\begin{aligned} \tfrac{dy}{dt} &= x(1+x)^{-2l-1} \equiv g(x) \\ \tfrac{dx}{dt} &= -y + \int\limits_0^x (mx+\delta)(1+x)^{-l-1} dx \equiv -y - F(x) \end{aligned} \tag{3.14}$$

As $m\delta l < 0$, we need to compute the divergence of (3.14), which is given by

$$\text{div}(3.14) = (mx+\delta)(1+x)^{-l-1} \tag{3.15}$$

Notice that the limit cycle can not touch the line $1 + x$ as $x > -1$. It must intersect with $mx + \delta = 0$ if the limit cycle exists, which implies a limit cycle can exist only if $\delta > m$. Then we complete the proof. □

The following theorem can be derived directly from Lemma 3.2.

Theorem 3.3 *When*

$$S_0 \leq \frac{1 - R + (1+k_d)\tau}{R - 1 + (1-k_d)\tau}$$

system (2.1) *with* $\beta = \gamma = 1$ *and* $X_0 = 0$ *or system* (3.5) *has no limit cycle surrounding the non-washout equilibrium,* E_2.

In what follows we shall investigate the existence of the limit cycle. By Lemma 3.2 we only need to focus on the parameter region where $\delta > m$. Consider system (3.9), We have

Lemma 3.3 *When* $\delta > \max\{m, -2\}$ *system* (3.9) *has an unique unstable limit cycle.*

Proof First from Theorem 3.2 and Lemma 3.2 we know that if the limit cycle exists, $\delta > \max\{m, -2\}$. Secondly, by using Theorem 16.8 of [19] or the results of Han [7], we can easily prove that the solution of system (3.9) is unbounded and the number of unbounded trajectories is greater than 2. Then, from Theorem 3.2 and its proof, the origin of (3.9) is stable. Therefore according to the Poincaré-Bendixson theorem we can conclude that there is a unstable limit cycle for system (3.9). At last we can see the limit cycle must be unique from Lemma 3.1. This completes the proof. □

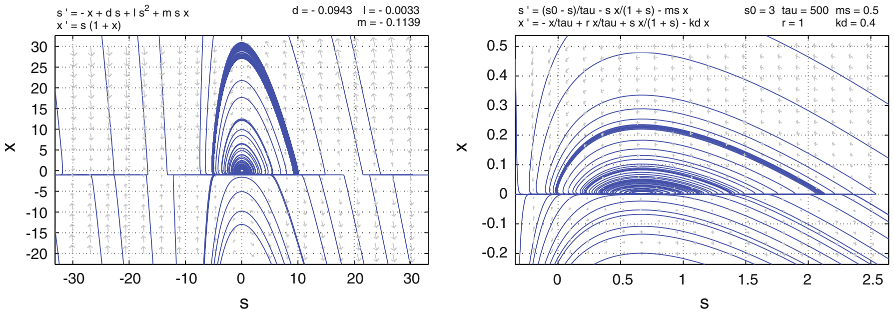

Fig. 2 Unstable limit cycle

4 Conclusion

In this paper, we carried out the qualitative analysis of models for a continuous bioreactor and a membrane reactor. The conditions for the existence, non-existence and uniqueness have been given. As the non-washout equilibrium is always stable and the system is unbounded, an unstable limit cycle can exist under certain condition. A numerical simulation has also been carried out, which supports our theoretical analysis, please see Fig. 2 for instance.

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