Available online at http://scik.org
Commun. Math. Biol. Neurosci. 2016, 2016:1
ISSN: 2052-2541

THEORETICAL ANALYSIS OF ETHANOL FERMENTATION WITH PRODUCT INHIBITION AND SYNCHRONOUS IMPULSE

ZHONG ZHAO[1,*] CHENGGUANG LUO[1], YI XIAO[2]

[1]Department of Mathematics, Huanghuai University Zhumadian 463000, Henan, China

[2]The Second Junior School of Zhumadian City, Zhumadian 463000, Henan, China

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Abstract. In this paper, a universal model of ethanol fermentation with product inhibition and synchronous impulse is investigated. Firstly, continuous input substrate is taken. By using the qualitative theory of ordinary differential equations, we prove the complex dynamics of the equilibria. Moreover, synchronous impulse of input substrate is also considered. Using small amplitude perturbation, we obtain the biomass-free periodic solution is locally stable if some conditions are satisfied. In a certain limiting case, it is shown that a nontrivial periodic solution emerges via a supercritical bifurcation. The above results are validated by numerical simulations.

Keywords: Saddle-node; Impulsive input; Periodic solution; Bifurcation.

2010 AMS Subject Classification: 92D40, 93C15, 34H15, 92B05.

1. Introduction

With the rapid development of the national economy, the explosion in the number of motor vehicles has caused serious air pollution. The development of fuel alcohol, not only can greatly reduce the content of harmful substances in vehicle exhaust, but also can solve the energy crisis. Furthermore, fuel alcohol may be obtained from the microorganism fermentation. during the

*Corresponding author

E-mail addresses: zhaozhong8899@163.com

Received February 8, 2015

microorganism fermentation, a major problem is the relatively low product yields and relatively low productivity because the fermentation process is affected by many factors[1-9]. To enhance the alcohol production, Wei[6] proposed a mathematical model of ethanol fermentation with gas stripping as follows:

$$\begin{cases} \dfrac{dS}{dt} = D(S^0 - S) - \dfrac{\mu S x}{\delta_1 (K_s + S)} - mx, \\ \dfrac{dx}{dt} = \dfrac{\mu S x}{K_s + S} - Dx, \\ \dfrac{dP}{dt} = \dfrac{\mu S x}{\delta_2 (K_s + S)} - (D + \beta_0)P, \end{cases} \tag{1.1}$$

x is the biomass concentration ; S is the substrate concentration ; S^0 is the initial substrate concentration; P is the ethanol concentration; D is the dilution rate; δ_1 and δ_2 are the cell yield coefficient and the production yield coefficient, respectively; μ is the maximum specific growth rate; m is the maintenance coefficient; β_0 is the stripping factor. K_s is the half-saturation constant.

The Monod model is only used when the presence of toxic metabolic products plays no inhibitory role. Therefore, we need to investigate the effect of substrate input on the production of ethanol. where μ is the maximal specific growth rate of biomass.

Based on [6,9], we consider the following mathematical model of the ethanol fermentation:

$$\begin{cases} \dfrac{dS}{dt} = D(S^0 - S) - \dfrac{\mu S x}{\delta_1 (K_s + S + S^2/k_1)} - mx, \\ \dfrac{dx}{dt} = \dfrac{\mu S x}{K_s + S + S^2/k_1} - Dx, \\ \dfrac{dP}{dt} = \dfrac{\mu S x}{\delta_2 (K_s + S + S^2/k_1)} - (D + \beta_0)P, \end{cases} \tag{1.2}$$

k_1 is the inhibition constant, reflecting the inhibition effect of high concentration substrate. Other parameter are the same as system (1.1)

We notice that the variable P does not appear in the first two equations of (1.2). This allows us to consider the following system:

$$\begin{cases} \dfrac{dS}{dt} = D(S^0 - S) - \dfrac{\mu k_1 S x}{\delta_1 (k_1 K_s + k_1 S + S^2)} - mx =: p(S)(\dfrac{D(S^0 - S)}{p(S)} - x), \\ \dfrac{dx}{dt} = \dfrac{\mu S x}{K_s k_1 + k_1 S + S^2} - Dx, \end{cases} \tag{1.3}$$

where $p(S) = \dfrac{k_1\mu S}{K_s k_1 + k_1 S + S^2} + m$. From the practical view of fermentation, we only consider system (1.3) in the positive region $S \geq 0, x \geq 0$.

2. Qualitative analysis of system (1.3)

Firstly, we prove the boundedness of system (1.3).

Theorem 2.1. *System (1.3) is ultimately bounded.*

Proof. Define a function $W(S,x) = \delta_1 S + x$. We compute the derivative of $W(S,x)$ along a solution of (1.3).

$$\dot{W}(S,x) \leq D\delta_1 S^0 - D\delta_1 S - Dx,$$

we have $\delta_1 S + x \to \delta_1 S^0$ as $t \to \infty$. The proof is completed.

We consider equilibrium solutions to exist only if they lie in the positive quadrant. System (1.3) has at most three equilibrium solutions. The equilibrium $E_0 = (S^0, 0)$ always lies on the $S-$axis, representing the extinction of the microorganism.

Let λ_1 and $\lambda_2 (\lambda_1 \leq \lambda_2)$ denote the two possible solutions of the quadratic equation $\dfrac{\mu k_1 S}{k_1 K_s + k_1 S + S^2} = D$. Whether zero, one, or both of these other equilibria exist and sit in the positive quadrant depends on the relative positions of the nutrient isocline $x = \dfrac{D(S^0 - S)}{\frac{\mu k_1 S}{K_s k_1 + k_1 S + S^2} + m}$ and the microorganism isocline $x = \lambda_1$ and $x = \lambda_2$.

From system (1.3), we have $\dfrac{\mu k_1 S}{k_1 K_s + k_1 S + S^2} = D$, which is equivalent to

$$S^2 + \frac{k_1(D-\mu)}{D} S + k_1 K_s = 0. \tag{2.1}$$

Therefore, system (2.1) has positive roots if $\Delta = \frac{{k_1}^2 (D-\mu)^2}{D^2} - 4k_1 K_s \geq 0$, that is, $\mu \geq \frac{D(k_1 + 2\sqrt{k_1 K_s})}{k_1}$.

Obviously, when $\mu > \dfrac{D(k_1 + 2\sqrt{k_1 K_s})}{k_1}$, system (1.3) has at most three equilibria $E_0(S^0, 0), E_{\lambda_1}(\lambda_1, x_1)$ and $E_{\lambda_2}(\lambda_2, x_2)$, where

$$\lambda_1 = \frac{k_1(\mu - D) - D\sqrt{\Delta}}{2D}, x_1 = \frac{D\delta_1(S^0 - \lambda_1)(K_s k_1 + k_1\lambda_1 + {\lambda_1}^2)}{\delta_1 m {\lambda_1}^2 + k_1(\delta_1 m + \mu)\lambda_1 + m k_1 K_s \delta_1}$$

$$\lambda_2 = \frac{k_1(\mu - D) + D\sqrt{\Delta}}{2D}, x_2 = \frac{D\delta_1(S^0 - \lambda_2)(K_s k_1 + k_1\lambda_2 + {\lambda_2}^2)}{m\delta_1 {\lambda_2}^2 + k_1(\delta_1 m + \mu)\lambda_2 + m k_1 K_s \delta_1}.$$

Next, we consider the possible phase portraits of system (1.3).

Theorem 2.2. *If* $\mu < \dfrac{D(k_1+2\sqrt{k_1K_s})}{k_1}$ *holds, then system (1.3) has no interior equilibria. It is easy to that equilibrium* $E_0(S^0,0)$ *is a stable node.*

The proof can be obtained through the characteristic roots of the variational matrix about $E_0(S^0,0)$. Hence, we omit it.

Theorem 2.3. *If* $\mu = \dfrac{D(k_1+2\sqrt{k_1K_s})}{k_1}$ *and* $S^0 > \sqrt{K_sk_1}$ *hold, then system (1.3) has two equilibria: a hyperbolic saddle* $(S^0,0)$ *and an interior equilibrium* (S^*,x^*)*, where* $S^*=\lambda_1=\lambda_2=\sqrt{K_sk_1}, x^*=\dfrac{D\delta_1(S^0-S^*)(K_sk_1+k_1S^*+S^{*2})}{m\delta_1S^{*2}+k_1(\delta_1m+\mu)S^*+mk_1K_s\delta_1}$. (S^*,x^*) *is a saddle-node if* $\Delta_0=\delta_1D(S^0-S^*)(k_1+2S^*)-k_1\mu(\delta_1S^*+x^*)-\delta_1mx^*(k_1+2S^*)\neq 0$.

Proof. First, $E_0(S^0,0)$ is a hyperbolic saddle, which is easy to prove. Next, we will prove (S^*,x^*) is a saddle-node. It is clear that the determinant of the matrix $J(S^*,x^*)$ is zero, therefore the equilibrium (S^*,x^*) is degenerate.

We first make the following transformation $dt=(K_sk_1+k_1S+S^2)d\tau$ and system (1.3) now takes the form:

$$\begin{cases} \dfrac{dS}{d\tau}=(D(S^0-S)-mx)(K_sk_1+k_1S+S^2)-\dfrac{k_1\mu}{\delta_1}Sx, \\ \dfrac{dx}{d\tau}=x(k_1(\mu-D)S-DK_sk_1-DS^2), \end{cases} \tag{2.3}$$

To determine the dynamics of system (1.3) in the neighborhood of the equilibrium (S^*,x^*), we again transform the equilibrium (S^*,x^*) of system (1.3) to the origin and expand the righthand side of system as a Taylor series.

$$\begin{cases} \dfrac{dX}{d\tau} = \Delta_0X-[m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*]Y \\ \qquad +[DS^0-3DS^*-mx^*-Dk_1]X^2-(k_1m+\frac{k_1\mu}{\delta_1}+2mS^*)XY-mX^2Y-DX^3, \\ \frac{dY}{d\tau}=-Dx^*X^2-DX^2Y=:\varphi(S,x), \end{cases} \tag{2.4}$$

where $\Delta_0=(DS^0-DS^*-mx^*)(k_1+2S^*)-k_1\mu(S^*+\frac{x^*}{\delta_1})$. Let

$$\begin{aligned} &\Delta_0X-[m(k_1K_s+k_1S^*+S^{*2})+\tfrac{k_1\mu}{\delta_1}S^*]Y \\ &+[DS^0-3DS^*-mx^*-Dk_1]X^2-(k_1m+\tfrac{k_1\mu}{\delta_1}+2mS^*)XY-mX^2Y-DX^3=0. \end{aligned} \tag{2.5}$$

We can find a function $X=f(Y)$, $X(0)=0$ since $\Delta_0\neq 0$. Without loss of generality, suppose

$$f(Y)=c_1Y+c_2Y^2+c_3Y^3+\cdots. \tag{2.6}$$

Substituting (2.5) into (2.4), we have $\Delta_0(c_1Y+c_2Y^2+c_3Y^3+\cdots)-[m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*]Y+[DS^0-3DS^*-mx^*-Dk_1](c_1Y+c_2Y^2+c_3Y^3+\cdots)^2-(k_1m+\frac{k_1\mu}{\delta_1}+2mS^*)(c_1Y+c_2Y^2+c_3Y^3+\cdots)Y-m(c_1Y+c_2Y^2+c_3Y^3+\cdots)^2Y-D(c_1Y+c_2Y^2+c_3Y^3+\cdots)^3=0$, by comparing the coefficient, $c_1=\dfrac{m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*}{\Delta_0}$. Hence we obtain $f(Y)=\dfrac{m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*}{\Delta_0}Y+\cdots$. From system (2.4), we get

$$\varphi(f(Y),Y)=-Dx^*(\frac{m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*}{\Delta_0}Y+\cdots)^2$$

$$-D(\frac{m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*}{\Delta_0}Y+\cdots)^2Y.$$

Therefore, $m=2, g=-Dx^*(\dfrac{m(k_1K_s+k_1S^*+S^{*2})+\frac{k_1\mu}{\delta_1}S^*}{\Delta_0})^2$, we have the equilibrium (S^*,x^*) is a saddle-node by [10].

The following lemma together with the Poincare criterion [11] will be useful to eliminate the possibility of the periodic orbits of system (1.3).

Lemma 2.4. *Let* Γ *be any periodic orbit of system (1.3). Then*

$$\Delta_1=\oint_\Gamma div(\dot{S},\dot{x})dt=\oint_\Gamma p(S)\frac{d}{dt}(\frac{D(S^0-S)}{p(S)})dt.$$

Proof.

$$\begin{aligned}
\Delta_1 &= \oint_\Gamma div(\dot{S},\dot{x})dt\\
&= \oint_\Gamma(-D-\frac{k_1\mu x(K_sk_1-S^2)}{\delta_1(K_sk_1+k_1S+S^2)^2)}+(\frac{k_1\mu S}{K_sk_1+k_1S+S^2}-D))dt\\
&= \oint_\Gamma(-D-\frac{k_1\mu(K_sk_1-S^2)}{\delta_1(K_sk_1+k_1S+S^2)^2)}\cdot\frac{D(S^0-S)-\dot{S}}{\frac{k_1\mu S}{\delta_1(K_sk_1+k_1S+S^2)+m}}+\frac{d}{dt}\ln x(t))dt\\
&= \oint_\Gamma[p(S)\frac{d}{dt}(\frac{D(S^0-S)}{p(S)})+\frac{d}{dt}\ln p(S)]dt\\
&= \oint_\Gamma p(S)\frac{d}{dt}(\frac{D(S^0-S)}{p(S)})dt.
\end{aligned}$$

Theorem 2.5. *When* $S^0<\lambda_1$ *and* $\mu>\frac{D(k_1+2\sqrt{k_1K_s})}{k_1}$, *system (1.3) has one microorganism-free equilibrium* $E_0(S^0,0)$, *which is a stable node and no interior equilibrium.*

The proof is clear and we omit it.

Theorem 2.6. *When $\lambda_1 < S^0 < \lambda_2$ and $\mu > \frac{D(k_1+2\sqrt{k_1K_s})}{k_1}$, system (1.3) has two equilibria $E_0(S^0,0)$ and $E_{\lambda_1}(\lambda_1,x_1)$. In this case*

(a) The equilibrium $E_0(S^0,0)$ is a saddle.

(b) The interior equilibrium (λ_1,x_1) is globally asymptotically stable. The phase portrait is given in Fig.1(a).

Proof. We can obtain the characteristic equation of the linearization of system (1.3) near the equilibrium $(S^0,0)$ as follows:

$$\det\begin{pmatrix} -D-\gamma & -m-\dfrac{k_1\mu S^0}{\delta_1(K_sk_1+k_1S^0+S^0)^2} \\ 0 & \dfrac{k_1\mu S^0}{K_sk_1+k_1S^0+S^{0^2}}-D-\gamma \end{pmatrix}=0.$$

Obviously, we have $\gamma_1=-1$, $\gamma_2=\frac{k_1\mu S^0}{K_sk_1+k_1S^0+S^{0^2}}-D>0$. Hence the equilibrium $E_1(S^0,0)$ is a saddle.

Next we will show the equilibrium $E_{\lambda_1}(\lambda_1,x_1)$ is globally asymptotically stable. The proof of the local stability is similar to (I), we can also obtain the characteristic equation of the linearization at $E_{\lambda_1}(\lambda_1,x_1)$ is

$$\gamma^2+(D+\frac{k_1\mu x_1(k_1K_s-\lambda_1{}^2)}{\delta_1(K_sk_1+k_1\lambda_1+\lambda_1{}^2)^2})\gamma+(m+\frac{k_1\mu\lambda_1}{\delta_1(K_sk_1+k_1\lambda_1+\lambda_1{}^2)})\frac{k_1\mu x_1(K_sk_1-\lambda_1{}^2)}{(K_sk_1+k_1\lambda_1+\lambda_1{}^2)^2}=0. \tag{2.7}$$

From system (2.1), $\lambda_1\lambda_2=K_sk_1$, we have $\lambda_1<\sqrt{K_sk_1}$. Therefore, we obtain that the equilibrium $E_{\lambda_1}(\lambda_1,x_1)$ is locally stable. From system (1.3) and the conditions, we note that if the periodic solution exist it must encircle the critical point E_{λ_1}. From (2.7), we can obtain the equilibrium E_{λ_1} lies on a downslope of the microorganism isocline. According to Lemma 2.4, the periodic solution is stable if it exists around E_{λ_1}, which is impossible. According to Poincare-Bendixson Theorem, limit ω of all the orbits must be an equilibrium. This implies that E_{λ_1} is globally asymptotically stable. The proof is completed.

Theorem 2.7. *When $\lambda_1 < \lambda_2 < S^0$ and $\mu > \frac{D(k_1+2\sqrt{k_1K_s})}{k_1}$, system (1.3) has three equilibria $E_0(S^0,0)$ $E_{\lambda_1}(\lambda_1,x_1)$ and $E_{\lambda_2}(\lambda_2,x_2)$. In this case*

(a) The equilibrium $E_0(S^0,0)$ is a stable node.

(b) The interior equilibrium (λ_1, x_1) is stable focus or node. The equilibrium (λ_2, x_2) is a saddle.

(c) System (1.3) has no closed orbits. The phase portrait is given in Fig.1(b).

The proof of (a) and (b) is easy to obtain. The proof of (c) is similar to Theorem 2.6, we omit it.

3. The model of impulsive input

With an impulsive input, the equation (1.3) becomes

$$\begin{cases} \dfrac{dS}{dt} = -DS - \dfrac{\mu k_1 Sx}{\delta_1 (K_s k_1 + k_1 S + S^2)} - mx, & \\ & t \neq nT, \\ \dfrac{dx}{dt} = \dfrac{\mu k_1 Sx}{K_s k_1 + k_1 S + S^2} - Dx, & \\ \Delta S = DS^0, & \\ & t = nT, \\ \Delta x = 0, & \end{cases} \tag{3.1}$$

where T is the impulsive period, $n = \{1, 2, \cdots\}$. Other parameters are the same meanings as system (1.2).

By the basic theories of impulsive differential equations [12,13], the solution of system (3.1) is unique and piecewise continuous in $(nT, (n+1)T], n \in N$ for any initial values in R^2_+.

Considering the following subsystem

$$\begin{cases} \frac{dS}{dt} = -DS, & t \neq nT, \\ S(t^+) = S(t) + DS^0, & t = nT. \end{cases} \tag{3.2}$$

We can find a unique positive periodic solution $\widetilde{S}(t) = \dfrac{DS^0 \exp(-D(t-nT))}{1-\exp(-DT)}, t \in (nT, (n+1)T]$. Similar to Zhao el at. [14], it can be shown that $\widetilde{S}(t)$ is globally asymptotically stable by using stroboscopic map.

As a consequence, system (3.1) always has a biomass-free periodic solution $(\widetilde{S}(t), 0)$.

Theorem 3.1. *The biomass-free periodic solution $(\widetilde{S}(t), 0)$ is locally stable if $R < 1$, where*

$$R = \frac{1}{DT} \int_0^T \frac{\mu k_1 \widetilde{S}(t)}{K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t)} dt.$$

Proof. The local stability of the periodic solution may be determined by considering the behavior of small amplitude perturbations of the solution. Define

$$S(t) = y(t) + \widetilde{S}(t), \;\; x(t) = z(t).$$

The linearization of the first and second equations of (3.1) can be written as:

$$\begin{pmatrix} \dot{y}(t) \\ \dot{z}(t) \end{pmatrix} = \begin{pmatrix} -D & -\frac{\mu k_1 \widetilde{S}(t)}{\delta_1 (K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t))} - m \\ 0 & \frac{\mu k_1 \widetilde{S}(t)}{K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t)} - D \end{pmatrix} \begin{pmatrix} y(t) \\ z(t) \end{pmatrix}. \tag{3.3}$$

Let $\phi(t)$ be the fundamental solution matrix, then $\phi(t)$ satisfies

$$\frac{d\phi(t)}{dt} = \begin{pmatrix} -D & -\frac{\mu k_1 \widetilde{S}(t)}{\delta_1 (K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t))} - m \\ 0 & \frac{\mu k_1 \widetilde{S}(t)}{K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t)} - D \end{pmatrix} \phi(t), \tag{3.4}$$

and $\phi(0) = I$ is the identity matrix. The linearization of the third and fourth equations of system (3.1) becomes

$$\begin{pmatrix} y(nT^+) \\ z(nT^+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y(nT) \\ z(nT) \end{pmatrix}.$$

Thus, the monodromy matrix of (3.4) is

$$M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \phi(T).$$

From (3.4), we have $\phi(T) = \phi(0) \exp \int_0^T A dt \triangleq \phi(0) \exp(\overline{A})$, where $\phi(0)$ is the identity matrix. Let λ_1, λ_2 be eigenvalues of matrix M then

$$\begin{aligned} \lambda_1 &= \exp(-DT < 1, \\ \lambda_2 &= \exp \textstyle\int_0^T ((\frac{\mu k_1 \widetilde{S}(t)}{K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t)} - D) dt). \end{aligned}$$

Therefore, all eigenvalues of M, namely, λ_i $(i = 1, 2)$ have absolute values less than one if and only if $R < 1$. That is,

$$R = \frac{1}{DT} \int_0^T \frac{\mu k_1 \widetilde{S}(t)}{K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t)} dt < 1.$$

According to the Floquet theorem [13], we have $(\widetilde{S}(t), 0)$ is locally asymptotically stable.

The proof is completed.

Remark 3.1. The biomass-free periodic solution $(\widetilde{S}(t),0)$ is unstable if

$$R=\frac{1}{DT}\int_0^T \frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t)}dt>1.$$

4. The bifurcation of a nontrivial periodic solution

In the following, we shall study the loss of stability phenomenon mentioned in Remark 3.1 and prove that it is due to the onset of nontrivial periodic solutions obtained via a supercritical bifurcation in the limiting case, that is,

$$\frac{1}{DT}\int_0^T \frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t)}dt=1.$$

In order to get this purpose, we shall employ a fixed point argument. We denote by $\Phi(t,U_0)$ the solution of the (unperturbed) system consisting of the first two equations of (3.1) for the initial data $U_0=(u_0^1,u_0^2)$; also, $\Phi=(\Phi_1,\Phi_2)$. We define the mapping $I_1,I_2:R^2\to R^2$ by

$$I_1(x_1,x_2)=x_1+DS^0,\;\; I_2(x_1,x_2)=x_2$$

and the mapping $F_1,F_2:R^2\to R^2$ by

$$F(x_1,x_2)=-Dx_1-\frac{\mu k_1x_1x_2}{\delta_1(K_sk_1+k_1x_1+{x_1}^2)}-mx_2,\; F_2(x_1,x_2)=\frac{\mu k_1x_1x_2}{K_sk_1+k_1x_1+{x_1}^2}-Dx_2.$$

Furthermore, let us define $\Psi:[0,\infty)\times R^2\to R^2$ by

$$\Psi(T,U_0)=I(\Phi(T,U_0));\; \Psi(T,U_0)=(\Psi_1(T,U_0),\Psi_2(T,U_0)).$$

It is easy to see that Ψ is actually the stroboscopic mapping associated to the system (3.1), which puts in correspondence the initial data at 0_+ with the subsequent state of the system $\Psi(T^+,U_0)$ at T_+, where T is the stroboscopic time snapshot.

We reduce the problem of finding a periodic solution of (3.1) to a fixed problem. Here, U ia a periodic solution of period T for (3.1) if and only if its initial value $U(0)=U_0$ is a fixed point for $\Psi(T,\cdot)$. Consequently, to establish the existence of nontrivial periodic solutions of (3.1), one needs to prove the existence of the nontrivial fixed points of Ψ.

We are interested in the bifurcation of nontrivial periodic solutions near $(\widetilde{S}(t),0)$. Assume that $X_0=(x_0,0)$ is a starting point for the trivial periodic solution $(\widetilde{S}(t),0)$, where $x_0=\widetilde{S}(0^+)$.

To find a nontrivial periodic solution of period τ with initial value X, we need to solve the fixed point problem $X = \Psi(\tau, X)$, or denoting $\tau = T + \widetilde{\tau}, X = X_0 + \widetilde{X}$,

$$X_0 + \widetilde{X} = \Psi(T + \widetilde{\tau}, X_0 + \widetilde{X}).$$

Let us define

$$N(\widetilde{\tau}, \widetilde{X}) = X_0 + \widetilde{X} - \Psi(T + \widetilde{\tau}, X_0 + \widetilde{X}) = (N_1(\widetilde{\tau}, \widetilde{X}), N_2(\widetilde{\tau}, \widetilde{X})). \tag{4.1}$$

At the fixed point $N(\widetilde{\tau}, \widetilde{X}) = 0$. Let us denote

$$D_X N(0,(0,0)) = \begin{pmatrix} a'_0 & b'_0 \\ c'_0 & d'_0 \end{pmatrix}.$$

It follows that

$$a'_0 = 1 - \exp(-DT) > 0, \tag{4.2}$$

$$b'_0 = \exp(-DT) \int_0^T (m + \frac{\mu k_1 \widetilde{S}(s)}{\delta_1 (K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s))}) \frac{\partial \Phi_2}{\partial x_2}(s, X_0) \exp(Ds) ds, \tag{4.3}$$

$$c'_0 = 0, \tag{4.4}$$

$$d'_0 = 1 - \exp(\int_0^T (\frac{\mu k_1 \widetilde{S}(s)}{K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s)} - D) ds). \tag{4.5}$$

(See Appendix A_1 for details). A necessary condition for the bifurcation of nontrivial periodic solutions near $(\widetilde{S}(t), 0)$ is then

$$\det[D_X N(0,(0,0))] = 0.$$

Since $D_X N(0,(0,0))$ is an upper triangular matrix and $1 - \exp(-DT) > 0$, it consequently follows that $d'_0 = 0$ is necessary for the bifurcation. It is easy to see that $d'_0 = 0$ is equivalent to $\frac{1}{DT} \int_0^T \frac{\mu k_1 \widetilde{S}(s)}{K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s)} ds = 1$. It now remains to show that this necessary condition is also sufficient. This assertion represents the statement of the following theorem, which is our main result.

Theorem 4.1. *A supercritical bifurcation occurs at* $\frac{1}{DT} \int_0^T \frac{\mu k_1 \widetilde{S}(s)}{K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s)} ds = 1$, *in the sense that there is* $\varepsilon > 0$ *such that for all* $0 < \widetilde{\varepsilon} < \varepsilon$ *there is a stable positive nontrivial periodic solution of (3.1) with period* $T + \widetilde{\varepsilon}$.

Proof. According to the above notations, we obtain that

$$\dim(Ker[D_X N(0,(0,0))]) = 1,$$

and a basis $(-b_0'/a_0', 1)$ in $Ker[D_X N(0,(0,0))]$. Then the equation $N(\widetilde{\tau}, \widetilde{X}) = 0$ is equivalent to

$$N_1(\widetilde{\tau}, \alpha Y_0 + zE_0) = 0, N_2(\widetilde{\tau}, \alpha Y_0 + zE_0) = 0,$$

where $E_0 = (1,0)$, $Y_0 = (-b_0'/a_0', 1)$. $\widetilde{X} = \alpha Y_0 + zE_0$ represents the direct sum decomposition of $\widetilde{X}$ using the projections onto $Ker[D_X N(0,(0,0))]$ (the central manifold) and $Im[D_X N(0,(0,0))]$ (the stable manifold).

Let us define

$$f_1(\widetilde{\tau}, \alpha, z) = N_1(\widetilde{\tau}, \alpha Y_0 + zE_0),\ f_2(\widetilde{\tau}, \alpha, z) = N_2(\widetilde{\tau}, \alpha Y_0 + zE_0).$$

Firstly, we see that

$$\frac{\partial f_1}{\partial z}(0,0,0) = \frac{\partial N_1}{\partial x_1}(0,(0,0)) = a_0' \neq 0.$$

Therefore, by the implicit function theorem, one may solve the equation $f_1(\widetilde{\alpha}, \alpha, z) = 0$ near $(0,0,0)$ with respect to z as a function of $\widetilde{\tau}$ and α, and find $z = z(\widetilde{\tau}, \alpha)$ such that $z(0,0) = 0$ and

$$f_1(\widetilde{\tau}, \alpha, z(\widetilde{\tau}, \alpha)) = N_1(\widetilde{\tau}, \alpha Y_0 + z(\widetilde{\tau}, \alpha)E_0) = 0. \tag{4.6}$$

Moreover,

$$\frac{\partial z}{\partial \alpha}(0,0) = -(\frac{\partial N_1(0,0)}{\partial x_1})^{-1}\frac{\partial N_1(0,0)}{\partial x_2} + \frac{b_0'}{a_0'} = 0.$$

Then $N(\widetilde{\tau}, \widetilde{X}) = 0$ if and only if

$$f_2(\widetilde{\tau}, \alpha) = N_2(\widetilde{\tau}, (-\frac{b_0'}{a_0'}\alpha + z(\widetilde{\tau}, \alpha), \alpha)) = 0. \tag{4.7}$$

The equation (4.7) is called the "determining equation" and the number of its solutions equals the number of periodic solutions of (3.1).

Let us denote

$$f(\widetilde{\tau}, \alpha) = f_2(\widetilde{\tau}, \alpha, z).$$

First, it is to see that $f(0,0)=N_2(0,(0,0)=0$. We determine the Taylor expansion of f around $(0,0)$. For this, we compute the first order partial derivatives $\frac{\partial f}{\partial \widetilde{\tau}}(0,0)$ and $\frac{\partial f}{\partial \alpha}(0,0)$ and observe that

$$\frac{\partial f}{\partial \widetilde{\tau}}(0,0)=\frac{\partial f}{\partial \alpha}(0,0)=0.$$

(See Appendix A_2 for the proof of this fact). Furthermore, it is observed in Appendix A_3 that

$$A=\frac{\partial^2 f}{\partial \widetilde{\tau}^2}(0,0)=0,\ B=\frac{\partial^2 f}{\partial \alpha \partial \widetilde{\tau}}(0,0),\ C=\frac{\partial^2 f}{\partial \alpha^2}(0,0),$$

and hence

$$f(\widetilde{\tau},\alpha)=B\alpha\widetilde{\tau}+C\frac{\alpha^2}{2}+o(\widetilde{\tau},\alpha)(\widetilde{\tau}^2+\alpha^2).$$

By denoting $\widetilde{\tau}=l\alpha$ (where $l=l(\alpha)$), we obtain that (4.7) is equivalent to

$$Bl+C\frac{l^2}{2}+o(\alpha,l\alpha)(1+l^2)=0.$$

Next, we consider two cases:

Case I Suppose $\frac{\partial^2 f}{\partial \alpha^2}(0,0)<0$ and $\frac{\partial^2 f}{\partial \alpha \partial \widetilde{\tau}}(0,0)>0$, by denoting $\widetilde{\tau}=l\alpha$ (where $l=l(\alpha)$), we obtain that (4.7) is equivalent to

$$Bl+C\frac{l^2}{2}+o(l\alpha,\alpha)(1+l^2)=0.$$

Since $B>0$ and $C<0$, this equation is solvable with respect to l as a function of α. Moreover, here $l\approx -2B/C>0$.

Case II Suppose $\frac{\partial^2 f}{\partial \alpha^2}(0,0)<0$ and $\frac{\partial^2 f}{\partial \alpha \partial \widetilde{\tau}}(0,0)<0$, by denoting $\widetilde{\tau}=l\alpha$ (where $l=l(\alpha)$), we obtain that (4.7) is equivalent to

$$Bl+C\frac{l^2}{2}+o(l\alpha,\alpha)(1+l^2)=0.$$

Since $B<0$ and $C<0$, this equation is solvable with respect to l as a function of α. Moreover, here $l\approx -2B/C<0$.

Case III Suppose $\frac{\partial^2 f}{\partial \alpha^2}(0,0)>0$ and $\frac{\partial^2 f}{\partial \alpha \partial \widetilde{\tau}}(0,0)<0$, by denoting $\widetilde{\tau}=l\alpha$ (where $l=l(\alpha)$). Similarly we have $l\approx -2B/C>0$.

Case IV Suppose $\frac{\partial^2 f}{\partial \alpha^2}(0,0)>0$ and $\frac{\partial^2 f}{\partial \alpha \partial \widetilde{\tau}}(0,0)>0$, by denoting $\widetilde{\tau}=l\alpha$ (where $l=l(\alpha)$). Similarly we have $l\approx -2B/C<0$.

This implies that there is a supercritical bifurcation to a nontrivial periodic solution near a period T which satisfies the sufficient condition for the bifurcation

$$\frac{1}{DT}\int_0^T \frac{\mu k_1 \widetilde{S}(s)}{K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s)} ds = 1.$$

It is noteworthy that since this periodic solution appears via a supercritical bifurcation, the nontrivial periodic solution is stable. That is, there is $\varepsilon > 0$ such that for all $0 < \alpha < \varepsilon$ there is a stable positive nontrivial periodic solution of (3.1) with period $T + \widetilde{\tau}(\alpha)$ which starts in $X_0 \pm \alpha Y_0 + z(\widetilde{\tau}(\alpha), \alpha)E_0$. Here, $X_0, Y_0, E_0, z, \widetilde{\tau}$ are as defined above.

5. Discussion

Ethanol is one of the most widest used and heaviest demanded chemical, which may possibly become the substitute for gasoline. To expand markets for larger scale applications of various types of industry, it is necessary to minimize the cost of the ethanol product and study an effective methods of enhancing the output of the ethanol. Therefore, the mathematical model is a prerequisite for investigating the dynamical behavior.

To understand the oscillatory behavior of an experimental fermentor using the method of the theoretical analysis, we incorporate continuous input substrate and impulsive input substrate, respectively. Firstly, by using the qualitative theory of ordinary differential equations, we prove the biomass-free equilibrium point is a stable node if $\mu < \frac{D + k_1 + 2\sqrt{K_s k_1}}{k_1}$. If $\mu = \frac{D + k_1 + 2\sqrt{K_s k_1}}{k_1}$, system (1.3) has two equilibria: $E_0(S^0, 0)$ is a hyperbolic saddle and (S^*, x^*) is saddle-node when $\Delta_0 = \delta_1 D(S^0 - S^*)(k_1 + 2S^*) - k_1\mu(\delta_1 S^* + x^*) - \delta_1 m x^*(k_1 + 2S^*) \neq 0$. From Theorem 2.6 we obtain that the interior equilibrium is globally asymptotically stable if $\mu > \frac{D + k_1 + 2\sqrt{K_s k_1}}{k_1}$ and $\lambda_1 < S^0 < \lambda_2$ (see FIGURE 1(a)). Theorem 2.7 shows that system (1.3) has no closed orbit and three equilibria: a boundary equilibrium $E_0(S^0, 0)$ is a stable node; two interior equilibria E_{λ_1} and E_{λ_2} is a node and saddle, respectively if $\mu > \frac{D + k_1 + 2\sqrt{K_s k_1}}{k_1}$ and $\lambda_1 < \lambda_2 < S^0$(see FIGURE 1(b)). Secondly, we consider the impulsive input substrate. From Theorem 3.1, we obtain that the biomass-free periodic solution $(\widetilde{S}(t), 0)$ is locally asymptotically stable (In FIGURE 2) if $R < 1$ and unstable if $R > 1$. Therefore, $R = 1$ is a critical value. Using the bifurcation theorem, we show that once a threshold condition is reached, a

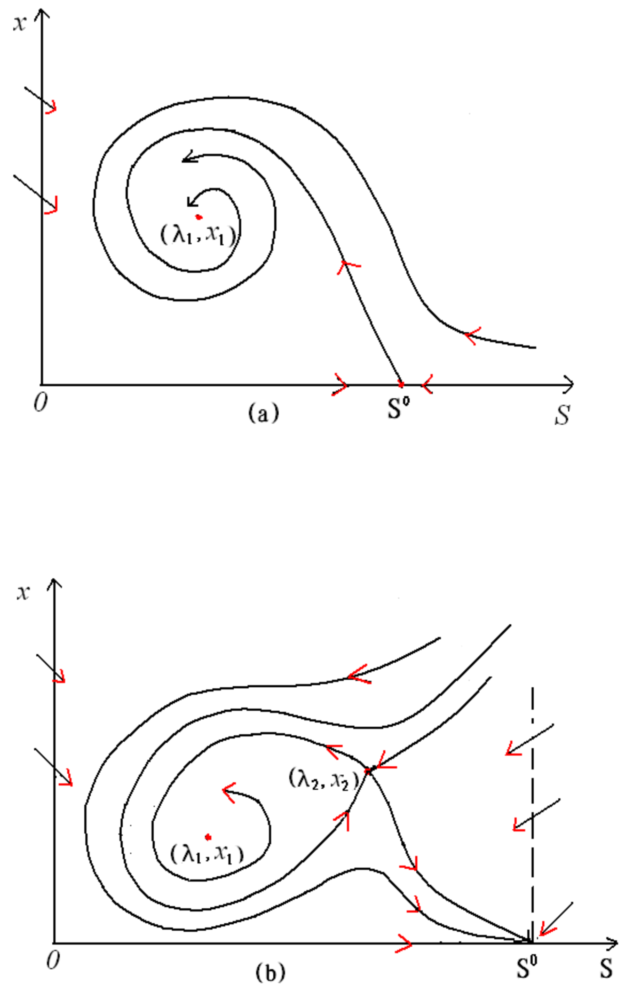

FIGURE 1. (a) The phase portraits of system (1.3) when $\mu > \frac{D(k_1+2\sqrt{k_1K_s})}{k_1}, \lambda_1 < S^0 < \lambda_2$. (b) The phase portraits of system (1.3) when $\mu > \frac{D(k_1+2\sqrt{k_1K_s})}{k_1}, \lambda_1 < \lambda_2 < S^0$.

stable nontrivial periodic solution emerges via a supercritical bifurcation, which is confirmed in FIGURE 3.

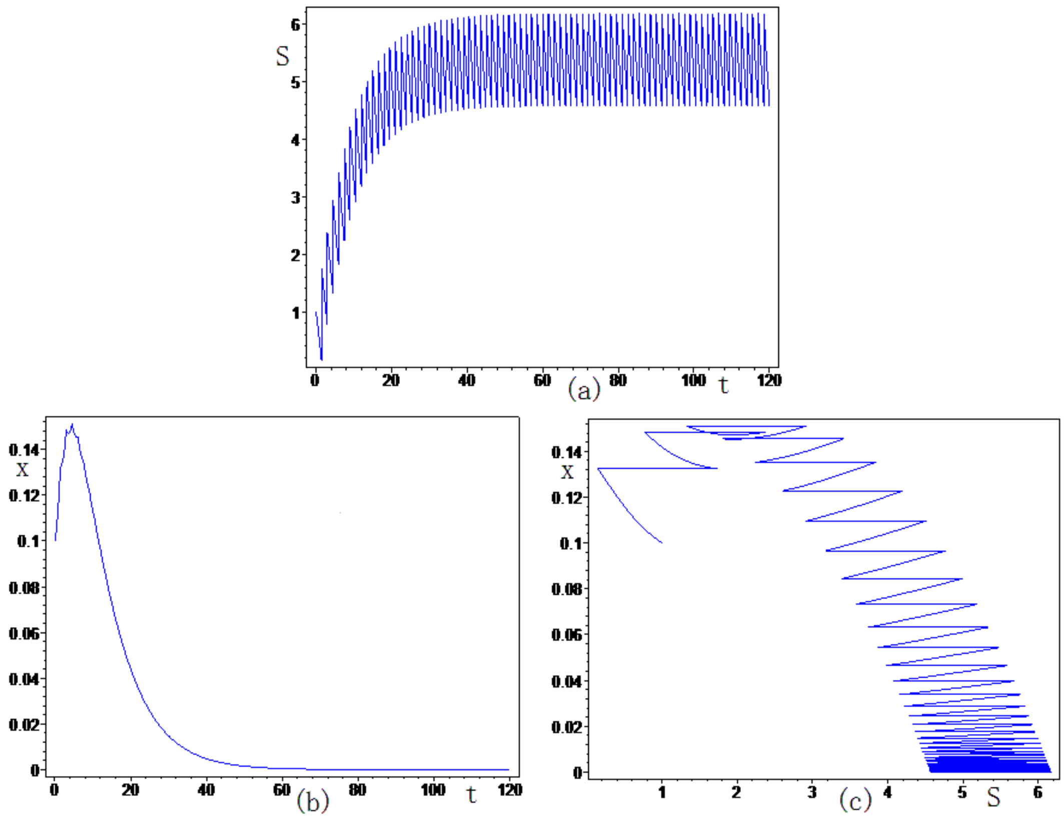

FIGURE 2. Dynamical behavior of system (1.3) with impulsive input with the parameters $S^0 = 8, D = 0.2, \mu = 1, \delta_1 = 0.1, m = 0.1, K_s = 0.2, k_1 = 0.5, T = 1.5, S(0) = 1, x(0) = 0.2$. (a) Time-series of the substrate concentration of system (1.3). (b) Time-series of the microorganism concentration of system (1.3). (c) Phase portrait of system (1.3).

Conflict of Interests

The authors declare that there is no conflict of interests.

Acknowledgements

This work is supported by the National Natural Science Foundation of China (No.11371164), NSFC-Talent Training Fund of Henan(U1304104), the backbone teacher of Henan(2013GGJS-214), Henan innovation talents in universities of science and technology plan(15HASTIT014) and Henan Science and Technology Department (122300410398, 132300410084 and 132300410250).

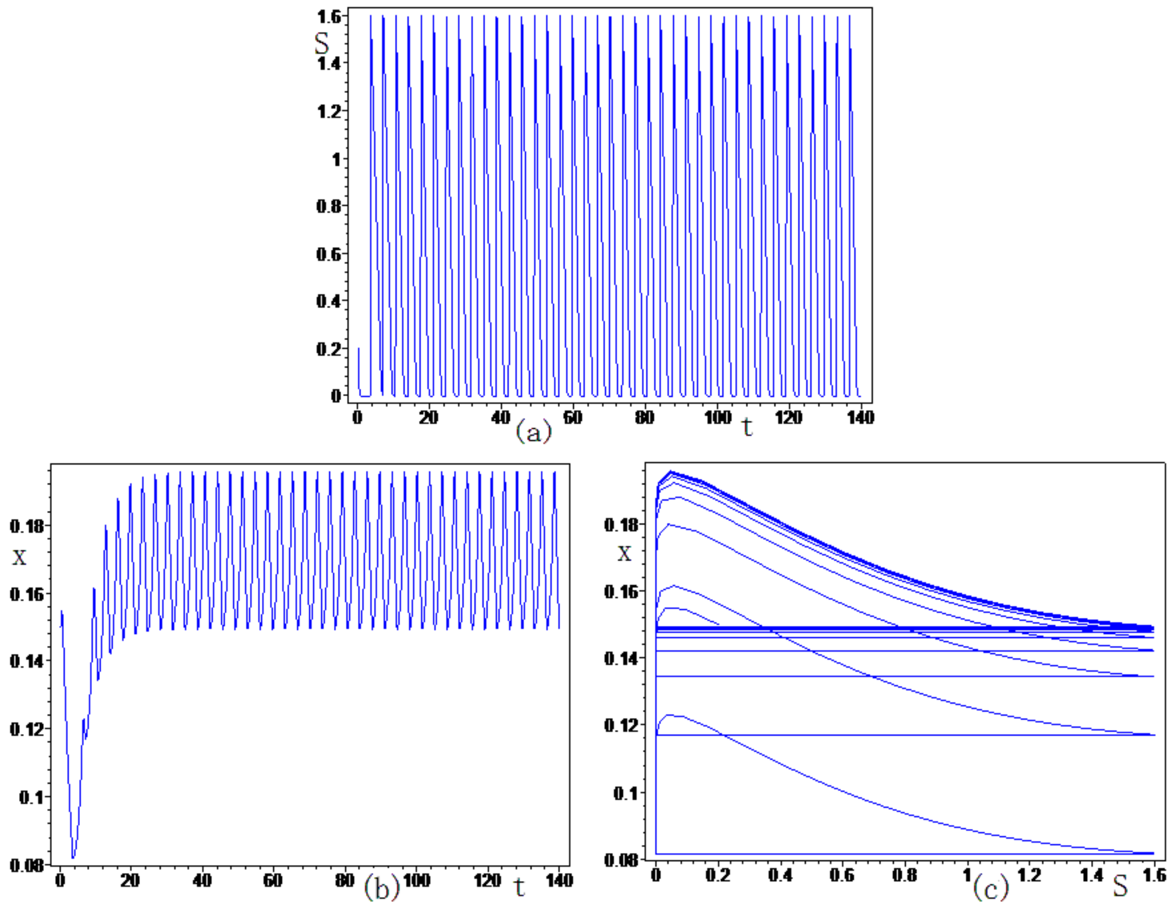

FIGURE 3. Dynamical behavior of system (1.3) with impulsive input with the parameters $S^0 = 8, D = 0.2, \mu = 1, \delta_1 = 0.1, m = 0.1, K_s = 0.2, k_1 = 0.5, T = 3.5, S(0) = 0.15, x(0) = 0.2$. (a) Time-series of the substrate concentration of system (1.3). (b) Time-series of the microorganism concentration of system (1.3). (c) Phase portrait of system (1.3).

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APPENDIX A. A

A.1. The first order partial derivatives of Φ_1, Φ_2. By formally deriving the equation

$$\frac{d}{dt}(\Phi(t,X_0)) = F(\Phi(t,X_0)),$$

which characterized the dynamics of the unperturbed flow associated to the first two equations in (3.1), one obtains that

$$\frac{d}{dt}[D_X\Phi(t,X_0)] = D_X F(\Phi(t,X_0))D_X\Phi(t,X_0). \tag{5.1}$$

This relation will be integrated in what follows in order to compute the components of $D_X\Phi(t,X_0)$ explicitly. Firstly, it is clear that

$$\Phi(t,X_0) = (\Phi_1(t,X_0),0).$$

Then we deduce that (5.1) takes the particular form

$$\frac{d}{dt}\begin{pmatrix} \frac{\partial\Phi_1}{\partial x_1} & \frac{\partial\Phi_1}{\partial x_2} \\ \frac{\partial\Phi_2}{\partial x_1} & \frac{\partial\Phi_2}{\partial x_2} \end{pmatrix}(t,X_0) = \begin{pmatrix} -D & -\frac{\mu k_1\widetilde{S}(t)}{\delta_1(K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t))} - m \\ 0 & \frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t)} - D \end{pmatrix}\begin{pmatrix} \frac{\partial\Phi_1}{\partial x_1} & \frac{\partial\Phi_1}{\partial x_2} \\ \frac{\partial\Phi_2}{\partial x_1} & \frac{\partial\Phi_2}{\partial x_2} \end{pmatrix}(t,X_0), \tag{5.2}$$

the initial condition for (5.2) at $t = 0$ being

$$D_X\Phi(0,X_0) = I_2. \tag{5.3}$$

Here, I_2 is the identity matrix in $M_2(R)$. It follows that

$$\frac{\partial\Phi_2(t,X_0)}{\partial x_1} = \exp(\int_0^t(\frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)} - D)ds)\frac{\partial\Phi_2(0,X_0)}{\partial x_1}.$$

This implies, using the initial condition (5.3), that

$$\frac{\partial\Phi_2(t,X_0)}{\partial x_1} = 0, \quad for \ \ t \geq 0. \tag{5.4}$$

To compute $\frac{\partial\Phi_1(t,X_0)}{\partial x_1}, \frac{\partial\Phi_1(t,X_0)}{\partial x_2}$ and $\frac{\partial\Phi_2(t,X_0)}{\partial x_2,}$. From (5.2) one obtain that

$$\frac{d}{dt}(\frac{\partial\Phi_1(t,X_0)}{\partial x_1}) = -D\frac{\partial\Phi_1(t,X_0)}{\partial x_1},$$

$$\frac{d}{dt}(\frac{\partial\Phi_1(t,X_0)}{\partial x_2}) = -D\frac{\partial\Phi_1(t,X_0)}{\partial x_2} - (m+\frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t})\frac{\partial\Phi_2(t,X_0)}{\partial x_2},$$

$$\frac{d}{dt}(\frac{\partial \Phi_2(t,X_0)}{\partial x_2}) = (\frac{\mu k_1 \widetilde{S}(t)}{K_s k_1 + k_1 \widetilde{S}(t) + \widetilde{S}^2(t)} - D)\frac{\partial \Phi_2(t,X_0)}{\partial x_2}.$$

According to the initial condition, we obtain that

$$\frac{\partial \Phi_1(t,X_0)}{\partial x_1} = \exp(-Dt),$$

$$\frac{\partial \Phi_1(t,X_0)}{\partial x_2} = -\exp(-Dt)\int_0^t (m + \frac{\mu k_1 \widetilde{S}(s)}{\delta_1(K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s))})\frac{\partial \Phi_2}{\partial x_2}(s,X_0)\exp(Ds)ds,$$

$$\frac{\partial \Phi_2(t,X_0)}{\partial x_2} = \exp(\int_0^t (\frac{\mu k_1 \widetilde{S}(s)}{K_s k_1 + k_1 \widetilde{S}(s) + \widetilde{S}^2(s)} - D)ds).$$

From (4.1), we obtain that

$$D_X N(0,(0,0)) = I_2 - D_X \psi(T,X_0),$$

which implies

$$D_X N(0,(0,0)) = \begin{pmatrix} a_0' & b_0' \\ 0 & d_0' \end{pmatrix}.$$

A.2. **The first order partial derivatives of f.**

$$\frac{\partial f}{\partial \alpha}(\widetilde{\tau},\alpha) = \frac{\partial}{\partial \alpha}(\alpha - \Psi_2(T+\widetilde{\tau}, X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0)) =$$
$$1 - (\frac{\partial \Phi_2}{\partial x_1}(T+\widetilde{\tau}), X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0)(-\frac{b_0'}{a_0'} + \frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha}) + \frac{\partial \Phi_2}{\partial x_2}(\widetilde{\tau}, X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0)),$$

but

$$\frac{\partial \Phi_2}{\partial x_1}(T+\widetilde{\tau}, X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0) = 0$$

and

$$d_0' = 1 - \frac{\partial \Phi_2}{\partial x_2}(T,X_0) = 0.$$

When $d_0' = 0$, then we obtain

$$\frac{\partial f}{\partial \alpha}(0,0) = 0.$$

On the other hand,

$$\begin{aligned} \frac{\partial f(\widetilde{\tau},\alpha)}{\partial \widetilde{\tau}} &= \frac{\partial}{\partial \widetilde{\tau}}(\alpha - \Psi_2(T+\widetilde{\tau}, X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0)) \\ &= -\frac{\partial \Phi_2}{\partial \widetilde{\tau}}(T+\widetilde{\tau}, X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0) - \frac{\partial \Phi_2}{\partial x_1}(T+\widetilde{\tau}, X_0 + \alpha Y_0 + z(\widetilde{\tau},\alpha)E_0). \end{aligned}$$

Since $\frac{\partial \Phi_2}{\partial x_1}(T+\widetilde{\tau}, X_0+\alpha Y_0+z(\widetilde{\tau},\alpha)E_0))=0$ and $\frac{\partial \Phi_2}{\partial \widetilde{\tau}}(T+\widetilde{\tau}, X_0+\alpha Y_0+z(\widetilde{\tau},\alpha)E_0))=0$. Therefore, we have $\frac{\partial f}{\partial \widetilde{\tau}}(0,0)=0$.

A.3. **Second partial derivatives of f.** Denote $A=\frac{\partial^2 f}{\partial \widetilde{\tau}^2}(0,0)$, $B=\frac{\partial^2 f}{\partial \widetilde{\tau}\partial \alpha}(0,0)$, $C=\frac{\partial^2 f}{\partial \alpha^2}(0,0)$.

Take $\eta(\widetilde{\tau})=T+\widetilde{\tau}, \eta_1(\widetilde{\tau},\alpha)=x_0-\frac{b_0'}{a_0'}+z(\widetilde{\tau},\alpha)$ and $\eta_2(\widetilde{\tau},\alpha)=\alpha$. Next we calculate these quantities in terms of the parameters of the equation.

Calculation of A

We have

$$
\begin{aligned}
\frac{\partial^2 f(\widetilde{\tau},\alpha)}{\partial \widetilde{\tau}^2} &= \frac{\partial^2}{\partial \widetilde{\tau}^2}(\eta_2 - I_2\circ\Phi(\eta,\eta_1,\eta_2))(\widetilde{\tau},\alpha)\\
&= -\frac{\partial^2}{\partial x_1^2}\Big(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}} + \frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big)^2\\
&\quad -\frac{\partial^2 I_2}{\partial x_1\partial x_2}\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}}\Big(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}} + \frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big)\\
&\quad -\frac{\partial^2 I_2}{\partial x_1\partial x_2}\frac{\partial \Phi_2}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}} + \frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big)\\
&\quad -\frac{\partial I_2}{\partial x_1}\Big(\frac{\partial^2 \Phi_1(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}^2} + 2\frac{\partial^2 \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1\partial \widetilde{\tau}}\frac{\partial z}{\partial \widetilde{\tau}}\Big)\\
&\quad -\frac{\partial I_2}{\partial x_1}\Big(\frac{\partial^2 \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1^2}\Big(\frac{\partial z}{\partial \widetilde{\tau}}\Big)^2 + \frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial^2 z}{\partial \widetilde{\tau}^2}\Big)\\
&\quad -\frac{\partial^2 I_2}{\partial x_2\partial x_2}\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}}\Big(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}} + \frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big)\\
&\quad -\frac{\partial^2 I_2}{\partial x_2\partial x_2}\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}}\frac{\partial z}{\partial \widetilde{\tau}}\Big(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}} + \frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big)\\
&\quad -\frac{\partial^2 I_2}{\partial x_2^2}\Big(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}} + \frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big)^2\\
&\quad -\frac{\partial I_2}{\partial x_2}\Big(\frac{\partial^2 \Phi_2(\eta,\eta_1,\eta_2)}{\partial \widetilde{\tau}^2} + 2\frac{\partial^2 (\eta,\eta_1,\eta_2)}{\partial x_1\partial \widetilde{\tau}}\frac{\partial z}{\partial \widetilde{\tau}}\Big)\\
&\quad -\frac{\partial I_2}{\partial x_2}\Big(\frac{\partial^2 \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1^2}\Big(\frac{\partial z}{\partial \widetilde{\tau}}\Big)^2 + \frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial z}{\partial \widetilde{\tau}}\Big).
\end{aligned}
$$

Since $\frac{\partial^2 I_2}{\partial x_2^2}=\frac{\partial \Phi_2}{\partial x_2}=\frac{\partial \Phi_2}{\partial \widetilde{\tau}}=\frac{\partial^2 \Phi_2}{\partial \widetilde{\tau}\partial x_1}=0$ for $(\widetilde{\tau},\alpha)=(0,0)$, then

$$
A=-\frac{\partial I_2}{\partial x_2}\frac{\partial^2 \Phi_2(T,x_0)}{\partial \widetilde{\tau}^2},
$$

on the other hand, we have $\frac{\partial^2 \Phi_2(t,X_0)}{\partial \widetilde{\tau}^2}=0$, therefore, we obtain $A=0$.

Calculation of C

We have

$$\frac{\partial^2 f}{\partial \alpha^2}(\widetilde{\tau},\alpha) = \frac{\partial^2}{\partial^2}(\eta_2 - I_2 \circ \Phi(\eta,\eta_1,\eta_2))$$

and

$$\begin{aligned}
\frac{\partial^2 f}{\partial \alpha^2}(\widetilde{\tau},\alpha) \quad &= -\frac{\partial^2 I_2}{\partial x_1^2}(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \widetilde{\tau}})+\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_2})^2 \\
&-\frac{\partial^2 I_2}{\partial x_1 \partial x_2}(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \widetilde{\tau}})-\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_2}) \\
&\times(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha})) \\
&-\frac{\partial^2 I_2}{\partial x_1 \partial x_2}(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha}))\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2} \\
&-\frac{\partial^2 I_2}{\partial x_1 \partial x_2}\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_2}\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2} \\
&-\frac{\partial I_2}{\partial x_1}(\frac{\partial^2 \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1^2}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha})^2) \\
&-2\frac{\partial I_2}{\partial x_1}\frac{\partial^2(\eta,\eta_1,\eta_2)}{\partial x_1 \partial x_2}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha}) \\
&-\frac{\partial I_2}{\partial x_1}(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}(\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha^2})^2+\frac{\partial^2 \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_2^2}) \\
&-\frac{\partial^2 I_2}{\partial x_1 \partial x_2}(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha})+\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_2}) \\
&\times(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha})) \\
&-\frac{\partial^2 I_2}{\partial x_1 \partial x_2}(\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha}))\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2} \\
&-\frac{\partial^2 I_2}{\partial x_1 \partial x_2}\frac{\partial \Phi_1(\eta,\eta_1,\eta_2)}{\partial x_2}\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2} \\
&-\frac{\partial^2 I_2}{\partial x_2^2}(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha})+\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2})^2 \\
&-\frac{\partial I_2}{\partial x_2}(\frac{\partial^2 \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1^2}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha})^2) \\
&-2\frac{\partial I_2}{\partial x_2}\frac{\partial^2 \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1 \partial x_2}(-\frac{b_0'}{a_0'}+\frac{\partial z(\widetilde{\tau},\alpha)}{\partial \alpha}) \\
&-\frac{\partial I_2}{\partial x_2}(\frac{\partial \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_1}\frac{\partial^2 z(\widetilde{\tau},\alpha)}{\partial \alpha^2}+\frac{\partial^2 \Phi_2(\eta,\eta_1,\eta_2)}{\partial x_2^2}).
\end{aligned}$$

On the one hand, for determining C, we must calculate the following terms:

$$\frac{\partial^2\Phi_2(T,X_0)}{\partial x_1\partial x_2},\frac{\partial^2\Phi_2(T,X_0)}{\partial x_2^2}.$$

We have

$$\frac{d}{dt}(\frac{\partial^2\Phi_2(t,X_0)}{\partial x_1\partial x_2})=(\frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t)}-D)\frac{\partial^2\Phi_2(t,X_0)}{\partial x_1\partial x_2}+\frac{\mu k_1(K_sk_1-\widetilde{S}^2(t))}{(K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t))^2}\frac{\partial\Phi_1(t,X_0)}{\partial x_1}\frac{\partial\Phi_2(t,X_0)}{\partial x_2}.$$

Since

$$\frac{\partial\Phi_2(0,X_0)}{\partial x_1\partial x_2}=0.$$

We obtain that

$$\frac{\partial^2\Phi_2(t,X_0)}{\partial x_1\partial x_2}=\exp(\int_0^t(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)\times\int_0^t\frac{\mu K_1(K_sk_1-\widetilde{S}^2(s))}{(K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s))^2}\frac{\partial\Phi_1(s,X_0)}{\partial x_1}ds.$$

Also, by a similar argument,

$$\frac{d}{dt}(\frac{\partial^2\Phi_2(t,X_0)}{\partial x_2^2})=(\frac{\mu k_1\widetilde{S}(t)}{K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t)}-D)\frac{\partial^2\Phi_2(t,X_0)}{\partial x_2^2}+\frac{\mu K_1(K_sk_1-\widetilde{S}^2(t))}{(K_sk_1+k_1\widetilde{S}(t)+\widetilde{S}^2(t))^2}\frac{\partial\Phi_1(t,X_0)}{\partial x_2}\frac{\partial\Phi_2(t,X_0)}{\partial x_2},$$

and since

$$\frac{\partial^2\Phi_2(0,X_0)}{\partial x_2^2}=0.$$

One may deduce that

$$\frac{\partial^2\Phi_2(t,X_0)}{\partial x_2^2}=\exp(\int_0^t(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)\ \int_0^t\frac{\mu k_1(K_sk_1-\widetilde{S}^2(s))}{(K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s))^2}\frac{\partial\Phi_1(s,X_0)}{\partial x_2}ds$$

Therefore, we have

$$\begin{aligned}C&=2\frac{b_0'}{a_0'}\cdot\frac{\partial^2\Phi_2(T,X_0)}{\partial x_1\partial x_2}-\frac{\partial^2\Phi_2(T,X_0)}{\partial x_2^2}\\&=2\frac{b_0'}{a_0'}\exp(\int_0^T(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)\times\int_0^T\frac{\mu k_1(K_sk_1-\widetilde{S}^2(s))}{(K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s))^2}\frac{\partial\Phi_1(s,X_0)}{\partial x_1}ds\\&-\exp(\int_0^T(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)\int_0^T\frac{\mu k_1(K_sk_1-\widetilde{S}^2(s))}{(K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s))^2}\frac{\partial\Phi_1(s,X_0)}{\partial x_2}ds.\end{aligned}$$

Similarly, we also obtain that

$$\begin{aligned}B&=-\left(\frac{\partial^2\Phi_2(T,X_0)}{\partial x_1\partial x_2}\cdot\frac{1}{a_0'}\cdot\frac{\partial\Phi_1(T,X_0)}{\partial\tilde{\tau}}+\frac{\partial\Phi_2(T,X_0)}{\partial\tilde{\tau}\partial x_2}\right)\\&=-((\exp(\int_0^T(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)\times\int_0^T\frac{\mu k_1(K_sk_1-\widetilde{S}^2(s))}{(K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s))^2}\frac{\partial\Phi_1(s,X_0)}{\partial x_1}ds\frac{1}{a_0'}\dot{\widetilde{S}}(T)\\&+(\frac{\mu k_1\widetilde{S}(T)}{K_sk_1+k_1\widetilde{S}(T)+\widetilde{S}^2(T)}-D)\exp(\int_0^T(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds))\\&=(\exp(\int_0^T(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)\times\int_0^T\frac{\mu k_1(K_sk_1-\widetilde{S}^2(s))}{(K_sK_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s))^2}\frac{\partial\Phi_1(s,X_0)}{\partial x_1}ds\frac{\widetilde{S}(T)}{a_0'}\\&-(\frac{\mu k_1\widetilde{S}(T)}{K_sk_1+k_1\widetilde{S}(T)+\widetilde{S}^2(T)}-D)\exp(\int_0^T(\frac{\mu k_1\widetilde{S}(s)}{K_sk_1+k_1\widetilde{S}(s)+\widetilde{S}^2(s)}-D)ds)).\end{aligned}$$