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DYNAMIC ANALYSIS OF ETHANOL, GLUCOSE, AND *SACCHAROMYCES* FOR BATCH FERMENTATION

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Abstract. In this paper, a dynamic model is presented to describe the behavior of glucose concentration, *Saccharomyces*, and ethanol concentration during batch fermentation process. The desired product of batch alcohol fermentation is ethanol. The form of this mathematical model is nonlinear differential equation systems. The equilibrium point stability of the dynamic model is discussed. Further, simulation numeric based on the experimental data is proposed to analysis the stability of dynamic model. From the simulations results, the behavior of glucose, *Saccharomyces*, and ethanol achieve steady-states at the 3rd day.

Keywords and Phrases : Dynamic model, ethanol, glucose, *Saccharomyces*, steady state

1. INTRODUCTION

A model for predicting alcoholic fermentation behaviour would be a valuable instrument for tequila research, due to the technical and economical implications has been proposed by Arellano-Plaza, et. al[1]. Some researchers [8] have presented a biochemically structured model for the aerobic growth of *Saccharomyces cerevisiae* on glucose and ethanol. They showed a bifurcation analysis using the two external variables, the dilution rate and the inlet concentration of glucose, as parameters, that a fold bifurcation occurs close to the critical dilution rate resulting in multiple steady states. Further, Wei and Chen [9] are investigated a mathematical model for ethanol fermentation with gas tripping. They studied the existence and local stability of two equilibrium points of the subsystem. Cheng-Ce Li [3] observed oscillations during the production of ethanol fermentation by *Zymomonas mobile*. The focus of their paper is to help understand which inhibitory mechanism mau cause the oscillatory phenomena in the fermentation proses. Furthermore, Widowati, et.al [11] proposed stability analysis of the dynamic model of alcoholic fermentation.

In comparison with previous papers [3, 9, 11], this paper investigates the dynamic analysis of batch alcoholic fermentation, whereas in [3, 9, 11] discussed the dynamic analysis of continuous alcoholic fermentation . In this paper, we present the stability analysis of the dynamic model of ethanol concentration, glucose concentration, and *Saccharomyces* during batch fermentation process. The local stability can be observed from the eigen values of the Jacobian matrix of the linearized system.

The paper is organized as follows. Section 2 describes mathematical modeling of alcoholic fermentation. Results concerning the stability analysis of the dynamic model are discussed in Section 3. In Section 4 the validity of the proposed method is presented by using experimental data. We demonstrate our results by numerical simulation. Finally, concluding remarks are given in Section 5.

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2. MATHEMATICAL MODELING

The process of fermentation is crucial in the ethanol production. The mathematical model is proposed to represent the dynamics of batch alcoholic fermentation. The model variables are glucose concentration, *Saccharomyces*, and ethanol concentration. The following set of differential systems describes a batch alcoholic fermentation process[5],

$$\begin{aligned} \frac{dP}{dt} &= \rho X, \\ \frac{dS}{dt} &= -qX, \\ \frac{dX}{dt} &= \frac{VS}{K+S}X, \end{aligned} \tag{1}$$

where ρ is the growth rate of ethanol (mg / ml), q is the rate of glucose consumption (mg / ml), P is concentration of ethanol (ml / ml), S is concentration of glucose (mg / ml), X is *Saccharomyces* wet weight (mg / ml), V is the maximal growth rate of *Saccharomyces* (mg / ml), K is Michaelis-Menten constant, $\rho \neq 0$ and $q \neq 0$.

Let the equilibrium $E(P^*, S^*, X^*)$ for ethanol, glucose, and Saccharomyces model system of equations (1). Equilibrium point can be obtained by

$$\frac{dP}{dt} = 0, \quad \frac{dS}{dt} = 0, \quad \frac{dX}{dt} = 0.$$

System of equations (1) at the point $E(P^*, S^*, X^*)$ can be written

$$\begin{aligned} \rho X^* &= 0 \\ -qX^* &= 0 \\ \frac{VS^*}{K+S^*}X^* &= 0 \end{aligned} \tag{2}$$

Further, we obtain equilibrium point, $E(P^*, S^*, X^*)$, of alcoholic fermentation model as follows

$$P^* = C, \quad S^* = \frac{aK}{V-a}, \quad X^* = 0, \tag{3}$$

where $\frac{VS^*}{K+S^*} = a$, $a \neq 0$.

2. STABILITY ANALYSIS

Stability analysis of dynamic models (1) is derived through linearized system around equilibrium point using Taylor series [2, 4, 7]. Local stability of the system around the equilibrium point can be determined by eigenvalues of the Jacobian matrix of the linearized system.

Consider,

$$\frac{dP}{dt} = W(P,S,X) = \rho X$$
$$\frac{dS}{dt} = Y(P,S,X) = -qX \tag{4}$$
$$\frac{dX}{dt} = Z(P,S,X) = \frac{VS}{K+S}X$$

where $\bar{P} = P - P^*$, $\bar{S} = S - S^*$ and $\bar{X} = X - X^*$.

Linearization model (4) in the equilibrium point $E(P^*,S^*,X^*)$ using Taylor series are as follows

$$\frac{d\bar{P}}{dt} = \frac{\partial W(P^*,S^*,X^*)}{\partial P}\bar{P} + \frac{\partial W(P^*,S^*,X^*)}{\partial S}\bar{S} + \frac{\partial W(P^*,S^*,X^*)}{\partial X}\bar{X}$$
$$\frac{d\bar{S}}{dt} = \frac{\partial Y(P^*,S^*,X^*)}{\partial P}\bar{P} + \frac{\partial Y(P^*,S^*,X^*)}{\partial S}\bar{S} + \frac{\partial Y(P^*,S^*,X^*)}{\partial X}\bar{X} \tag{5}$$
$$\frac{d\bar{X}}{dt} = \frac{\partial Z(P^*,S^*,X^*)}{\partial P}\bar{P} + \frac{\partial Z(P^*,S^*,X^*)}{\partial S}\bar{S} + \frac{\partial Z(P^*,S^*,X^*)}{\partial X}\bar{X}$$

Substitution (4) into the equation (5), so that we find

$$\frac{d\bar{P}}{dt} = \rho\bar{X} \tag{6}$$

$$\frac{d\bar{S}}{dt} = -q\bar{X}$$

$$\frac{d\bar{X}}{dt} = \frac{VX^*K}{(K+S^*)^2}\bar{S} + \frac{VS^*}{K+S^*}\bar{X}$$

System (6) in matrix form will become

$$\begin{bmatrix} \frac{d\bar{P}}{dt} \\ \frac{d\bar{S}}{dt} \\ \frac{d\bar{X}}{dt} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \rho \\ 0 & 0 & -q \\ 0 & \frac{VX^*K}{(K+S^*)^2} & \frac{VS^*}{K+S^*} \end{bmatrix} \begin{bmatrix} \bar{P} \\ \bar{S} \\ \bar{X} \end{bmatrix}, \tag{7}$$

with Jacobian matrix is

$$J = \begin{bmatrix} 0 & 0 & \rho \\ 0 & 0 & -q \\ 0 & \frac{VX^*K}{(K+S^*)^2} & \frac{VS^*}{K+S^*} \end{bmatrix}. \tag{8}$$

The behavior of the system (4) around the equilibrium point $\left(c, \frac{aK}{V-a}, 0\right)$ can be seen from the Jacobian matrix as follows:

$$J\left(C, \frac{aK}{V-a}, 0\right) = \begin{bmatrix} 0 & 0 & \rho \\ 0 & 0 & -q \\ 0 & 0 & a \end{bmatrix}.$$

Characteristic matrix equation $J\left(c, \frac{aK}{V-a}, 0\right)$ can be found by

$det\left(J\left(c, \frac{aK}{V-a}, 0\right) - \lambda I\right) = 0,$ where *I* is the identity matrix, so that we get

$$J\left(c, \frac{aK}{V-a}, 0\right) = \begin{vmatrix} -\lambda & 0 & \rho \\ 0 & -\lambda & -q \\ 0 & 0 & a-\lambda \end{vmatrix}.$$

The characteristic equation of matrix $J\left(c, \frac{aK}{V-a}, 0\right)$ is

$$(-\lambda)(-\lambda)(a-\lambda) = 0 \tag{9}$$

Equation (9) has solutions $\lambda_{1,2} = 0$ and $\lambda_3 = a$. It is indicate that the behaviour of the system around the equilibrium point $E(P^*,S^*,X^*)$ will be stable if $\lambda_3 \leq 0$. In this case, it should be $a \leq 0$ and the behaviour of the system around the equilibrium point $E(P^*,S^*,X^*)$ is unstable if $\lambda_3 > 0$. In this case $a > 0$. From the above results, the stability of equilibrium point $E(P^*,S^*,X^*)$ is determined by the eigenvalues of the Jacobian matrix.

3. NUMERICAL SIMULATION

As a verification of the proposed method is given numerical simulations using data from laboratory experiments. Here, we check the optimal concentration of ethanol and the stability of the system. We use data from Widowati, et al [10] which has been conducting experiments in the Microbiology laboratory for batch systems. The data consist of the concentration of ethanol, glucose 10%, and *Saccharomyces* wet weight. Further, by using the least square method and some manipulating algebra, we find the parameters $\rho = 1.3455$, $q = 0.011129$, $V = 0.087$, $K = 0.0628$.

Substituting these parameters in the equation (1), we have

$$\frac{dP}{dt} = 1.3455X$$
$$\frac{dS}{dt} = -0.011129X$$

$$\frac{dX}{dt} = \frac{0.087SX}{0.0628 + S} \tag{10}$$

Linearization of the system (10) around equilibrium point (P^*, S^*, X^*), $P^* = C$, $S^* = \frac{0.0628a}{0.087-a}$, $X^* = 0$, using Taylor series results the following equations

$$\frac{d\bar{P}}{dt} = 1.3455\bar{X}$$

$$\frac{d\bar{S}}{dt} = -0.011129\bar{X} \tag{11}$$

$$\frac{dX}{dt} = \frac{0.005464X^*}{(0.0628 + S^*)^2}\bar{S} + \frac{0.087S^*}{0.0628 + S^*}\bar{X},$$

Based on the data of ethanol, glucose, and Saccharomyces wet weigh [10], we obtain the Jacobian matrix,

$$J = \begin{bmatrix} 0 & 0 & 1.3455 \\ 0 & 0 & -0.011129 \\ 0 & 0 & -1.86 \end{bmatrix}.$$

Eigenvalues of the matrix J is as follows

$$\lambda_1 = \lambda_2 = 0 \text{ and } \lambda_3 = -1.86.$$

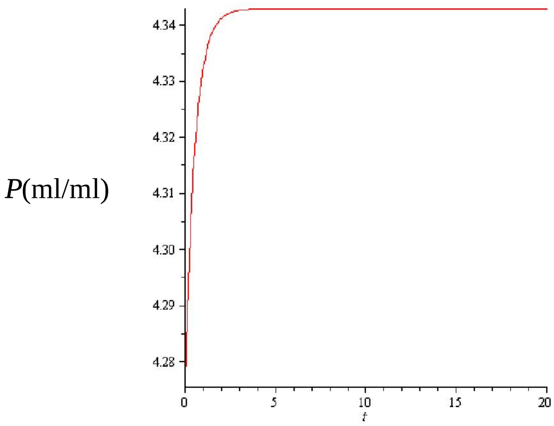
Solving the differential equation systems (11) using initial values, $\bar{P}(0) = 4.276, \bar{S}(0) = 0.3185, \bar{X}(0) = 0.092,$

are obtained particular solutions as follows

$$\bar{P} = 4.343 - 0.067e^{-1.86t}$$

$$\bar{S} = 0.3179 + 0.0006e^{-1.86t}$$
$$\bar{X} = 0.093e^{-1.86t}$$

Furthermore, we evaluate the behavior of the dynamic model around the equilibrium point.



day

Figure 1. Ethanol concentration vs time

S(mg/ml)

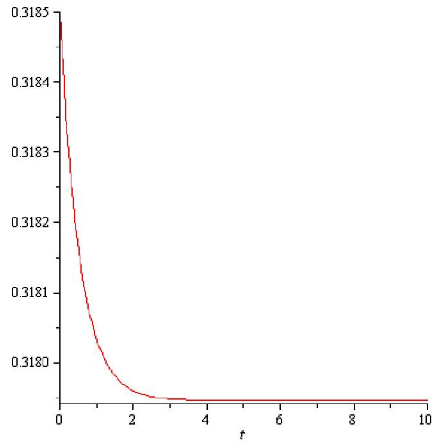


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Figure 2. Glucose concentration vs time

X (mg/ml)

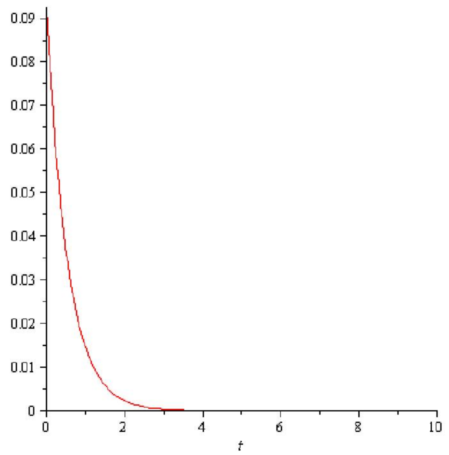

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Figure 3. *Saccharomyces* vs time

From Figure 1- 3, it can be seen that the ethanol concentration, glucose concentration, and *Saccharomyces* will achieve steady states. On the 3rd day, glucose concentration decrease and the number of *Saccharomyces* cells will reduce because no nutrients are consumed. It indicate that the fermentation process stops and the optimal concentration of ethanol is achieved at 3rd day.

4. CONCLUDING REMARK

Dynamic model have been proposed to describe the behavior of glucose concentration, S*accharomyces*, and ethanol concentration during batch fermentation process. Dynamical behavior around the equilibrium point is stable, if all of the real eigen values of the Jacobian matrix of the linearized system are less than or equal to zero. While the dynamical behavior of the systems around the equilibrium point is unstable if there exists a real part of the Jacobian matrix eigen value is greater than zero.

From the simulation results are found that the ethanol concentration, glucose concentration, and *Saccharomyces* will achieve steady states. It means that the dynamic model is stable. In this case, the optimal concentration of ethanol is achieved at 3rd day with glucose concentration 10%.

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