PERIODIC AND CHAOTIC SOLUTIONS FOR A MODEL OF A BIOREACTOR WITH CELL RECYCLE

S. Zaki, O. Saleh and G. Ibrahim

Basic Engineering Science Departement, Faculty of Engineering,
Menoufia University, Egypt
E-mail: gamal_i_m_a@yahoo.com

ABSTRACT

Modeling of bioreactor with cell recycle based on a pseudo-homogeneous floc model is proposed to predict complex dynamic behavior. The model is based on interactive kinetics between substrate and dissolved oxygen, and takes into account the external mass transfer resistance around the biological floc. The investigation of the static and dynamic bifurcation of the model shows that periodic as well as non-periodic behavior occur for some range of feed conditions and dissolved oxygen levels, as confirmed by several experiments studies reported in the literature. The ability of the proposed model to predict periodic behavior is investigated over a wide range of model parameters.

INTRODUCTION

Microbial cultures of *saccharomyces cerevisiae* and *Zymomonas mobilis,* two industrially important organisms are known to exhibit oscillatory behavior for some range of bioreactor parameters[1]. The occurrence of thses oscillations adversely affects control and optimize the operation of continuous bioreactors. While the mechanisms of these oscillations are not yet fully understood several theoretical and experimental studies have been reported in literature [2], [3] on the causes of this complex dynamic behavior.

One important experimental finding is the influence of dissolved oxygen levels on the occurrence of the periodic behavior. Porro[4] for instance examined the occurrence of spontaneous oscillations in the continuous cultures of the budding yeast, *S. cerevisiae*, and found that periodic behavior is strongly dependent on the dissolved oxygen levels.

This oscillatory behavior was explained by the oxidofermentative metabolism , which is supposed to be partly responsible for the spontaneous oscillations. the oscillations are related to a condition of growth in 'limiting' oxygen supply that doesn't allow a fully respiratory metabolism of glucose during specific phases of the cell recycle.

Parulekar [5] on the other hand confirm that changing dissolved oxygen levels can eliminate oscillations in continuous cultures of S.cerevisiae. The authors suggested that the oscillations could be elimiminated by raising or lowering dissolved oxygen levels above or below some critical values.

Sonnleitnert and Käppli [6] presented a model for the growth of baker's yeast on glucose. This model allows the prediction of experimental data without parameter adaption in biological dubious manner.

Ibrahim and Ajbar [7] proposed a pseudo-homogeneous dynamic floc model that predicts oscillatory behavior in microbial cultures. The floc model is based on the interactive kinetics between dissolved oxygen and the substrate. The model also takes into account the external mass transfer resistance around the biological floc. A static and dynamic investigation is then carried out for the proposed model.

In the contribution we use the model of Ibrahim and Ajbar as a microscopic model for a bioreactor with cell recycle and the complex dynamics of the system have been investigated.

MODEL RATIONALE

We consider the biomass i.e. bacterial floc as a catalyst pellet where the inter-particle diffussion is neglected i.e. perfectly mixed floc. Substrate and oxygen are being transported from the bulk solution to the surface of the bacterial floc. Once the materials reach the surface, physical and chemical interacions occur that produce the desired products.

Oxygen, playing an important role, has to be transported from the gas phase to the surface of the solid phase i.e. biological floc. Assumming good agitation that minimizes the bulk-liquid resistance, the transport of oxygen encounters two main resistance: a liquid-film resistance between the gas- liquid interface and the bulk of the liquid, and a liquid-film resistance at the solid interface. The two resistances are lumped into an overall mass resistance.

External mass transfer resistance plays in fact the role of delaying the reaction at the surface of the floc[8]. Some authors [9], [10] have analyzed the delaying effect and it was suggested that it could be the cause of periodic behavior in continuous cultures, where the inhibitory action of a compound is delayed. The delaying process is proposed in this contribution, however, is not due to the existence of an intermediate compound that inhibits the formation of the final product but rather to the existence of diffusion limitations and the delaying effect caused by interactive kinetics between oxygen and substrate as it will be shown later. This delaying effect seems quite natural since the fermentation medium is a heterogeneous one.

The model kinetic expressions are based on interactive kinetics between substrate and oxygen. The substrate (S) is consumed according to the following kinetic expressions

$$\mu = \mu_p + \mu_m \tag{1}$$

where μ_p is given by

$$\mu_p = \frac{\bar{\mu}\, S}{(K_s + S + S^2 / K_i)} \tag{2}$$

The maximum substrate consumption rate μ is assumed to be dependent on the oxygen concentration C and is given by

$$\bar{\mu} = \frac{\mu_{m1}\, \mathrm{C}}{(K_c + C)} \tag{3}$$

The term μ_p accounts then the interactive kinetics between oxygen and the substrate. Moreover it is clear from the expression adopted for μ that oxygen inhibits the maximum specific substrate consumption rate and hence plays a delaying effect on the reaction. Under aerobic conditions with oxygen in excess i.e. C taking the large rate expression μ_p becomes

$$\mu_p = \frac{\mu_{m1}\, S}{(K_s + S + S^2 / K_i)} \tag{4}$$

Which is the classical Haldane kinetic expression that accounts for substrate inhibition. Substrate inhibition kinetic has been recognized as fundamental in predicting the steady state multiplicity and the hysteresis phenomenon found experimentaly in bioreactors.

The second term μ_m for the kinetic expressions is given by

$$\mu_m = \frac{\mu_{m2}\, \mathrm{S}}{(K_x + S)} \tag{5}$$

The term μ_m represents the maintenance term. It accounts for the consumption of the substrate regardless of the respiration process. The classical Monod's expression is chosen for the maintenance term where K_x is the half saturation constant.

Floc Model

Having established the kinetics expressions . The unsteady state mass around the biological floc is drived in the following

1. Substrate

The mass transfer flux rate of substrate from bulk liquid concentration S_B to the surface concentration S_s is

$$N_s = K_{gs} A_c (S_B - S_s) \tag{6}$$

where A_c is the surface area of the floc and K_{gs} is the overall resistance for the substrate.

The unsteady mass balance equation for the consumption of the substrate in the floc of volume V_c is then

$$K_{gs}A_c(S_B - S_s) = \rho V_c\mu + V_c\frac{dS_s}{dt} \tag{7}$$

Recasting the expression of the consumption rate μ, Equation (7) becomes:

$$K_{gs}A_c(S_B - S_s) = \rho V_c\mu + \rho V_c\mu_p + V_c\frac{dS_s}{dt} \tag{8}$$

2. Oxygen

Oxygen is transferred from bulk gas to the surface of the biological floc where it is consumed with rate $\frac{\mu_p}{Y_{os}}$ where Y_{os} is the yield, assumed constant. Similarly to the substrate the unsteady state balance around the floc for oxygen is:

$$K_{gs}(C_B - C_s) = \rho V_c\frac{\mu_p}{Y_{os}} + V_c\frac{dC_s}{dt} \tag{9}$$

Reactor Model

A schematic diagram of the bioreactor with cell recycle is shown in Figure (1). The purge fraction W is operated directly from the reactor. Ideal conditions are assumed to prevail in the settler. Under these conditions the unsteady mass balance equation around the reactor for the different species are established in the following.

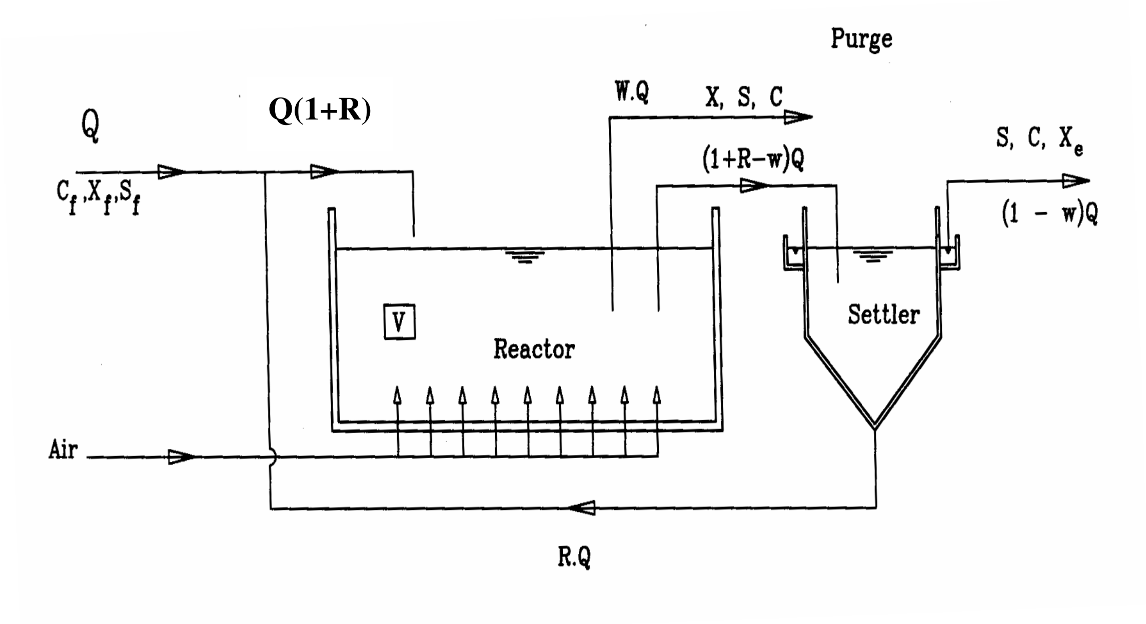


Figure (1) schematic diagram of the CSTBR with cell recycle

1. Biomass
Ideal conditions in the settler allows a simple relation between the recycle concentration X_R and the effluent concentration X:

$$X_R = X \frac{(1 + R - W)}{R} \tag{10}$$

where R is the recycled stream from the settler.

A mass balance around the reactor yields the following equation :

$$\frac{WX}{\theta} + \frac{dX}{dt} = \frac{X_f}{\theta} + \frac{S_s C_s X \mu_m}{(K_s + S_s + K_i S_s^2)(K_c + C_s)} \tag{11}$$

where $\theta = \frac{V}{Q}$ is the reactor residence time, X_f is the biomass feed concentration in mg/l.

2. Substrate
Similarly to the biomass mass balance equation, the equation of the substrate is as the following:

$$\frac{dS_B}{dt} = \frac{S_B \frac{dX}{dt}}{R - X} + \frac{R - X_f}{R - X}\left(\frac{S_f}{\theta}\right) - \frac{R - WX}{R - X}\left(\frac{S_B}{\theta}\right) - \frac{d_c K_{gs} X (S_B - S_S)}{R - X} \tag{12}$$

where S_f is the substrate feed concentration in mg / l.

3. Oxygen
Similarly to the substrate, the unsteady state balance around the reactor for oxygen is:

$$\frac{dC_B}{dt} = \frac{C_B \frac{dX}{dt}}{R - X} + \frac{R - X_f}{R - X}\left(\frac{C_f}{\theta}\right) - \frac{R - WX}{R - X}\left(\frac{C_B}{\theta}\right) - \frac{d_c K_{gc} X (C_B - C_S)}{R - X} + K_{la}(C^* - C_B) \tag{13}$$

where C_f is the oxygen feed concentration and K_{la} is the floc diameter.

Equations (8, 9, 11, 12 and 13) represents the autonomus model containing the system parameters. The nominal values of these parameters, chosen in the investigation are given in Table (1), The residence time (seta) is chosen as the bifurcation parameter.

RESULTS AND DISCUSSION

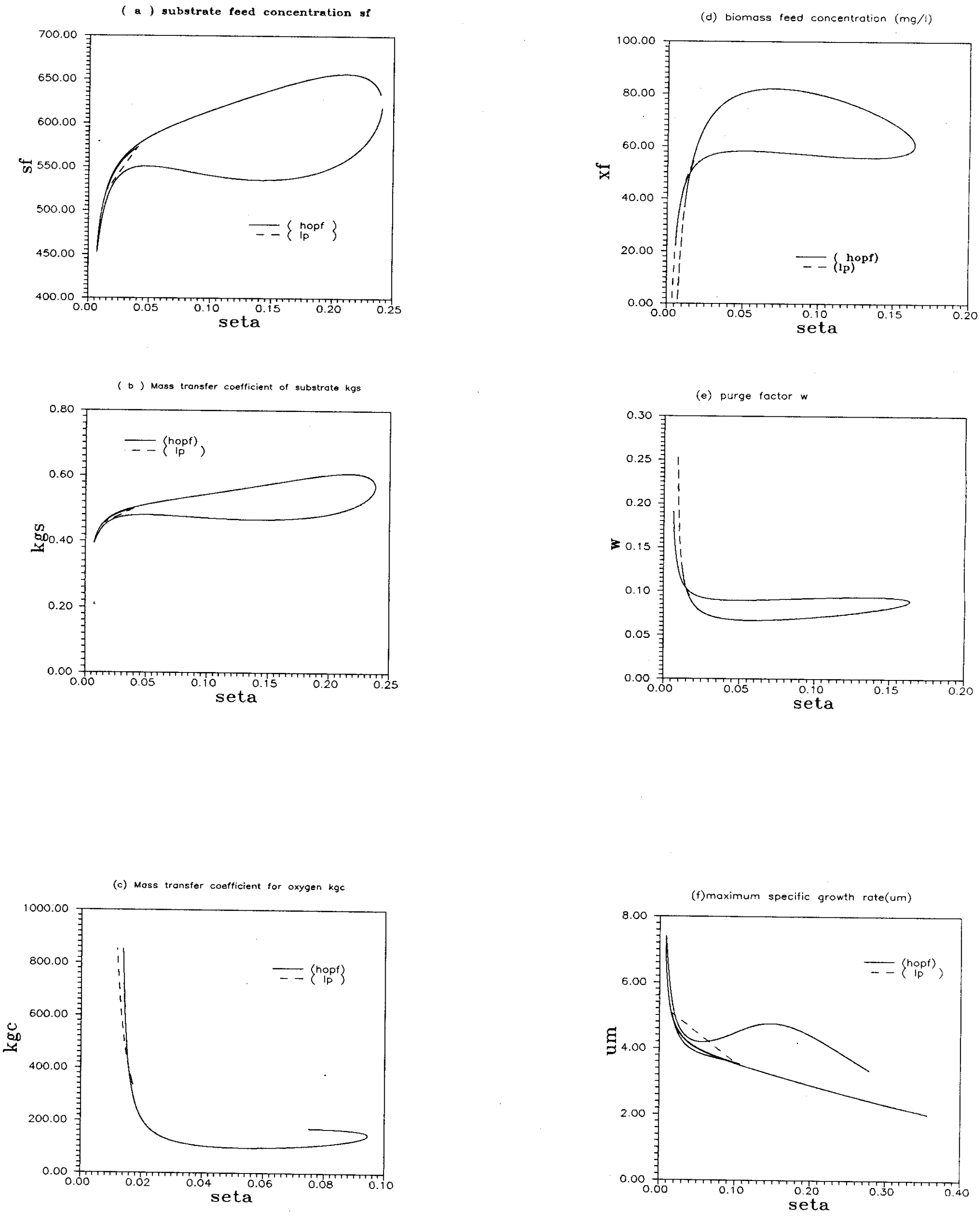
The bifurcation analysis is concerned with the way that steady state solutions of the model equations vary with the one of several system parameters. The residence time θ is the easiest parameter to vary and is selected to be the *bifurcation parameter*- main free parameter.

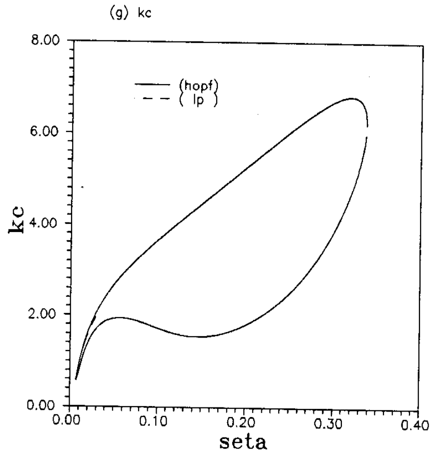
The continuity diagrams for some of the model parameters (kla, akgc, aki, akgs, kc, um, sf, df, xf, ms, akm, w) are shown in Figures (2-a, b, c, d, e, f, g, h, i, j, k, l).

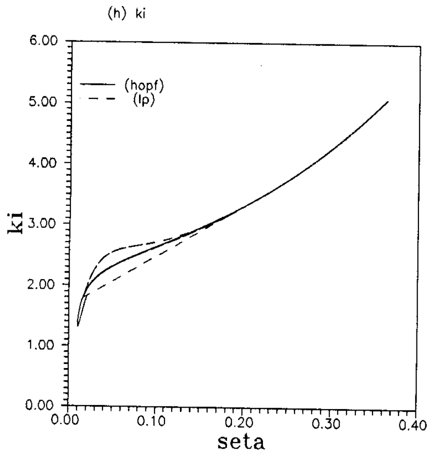
Diagrams show the loci of Hopf bifurcation points and limit point as the system parameters vary with residence time. These entire figures shows the presence of more than one HB point along a wide range of the system parameters. That means oscillation behavior (periodic or non-periodic) occurrence.

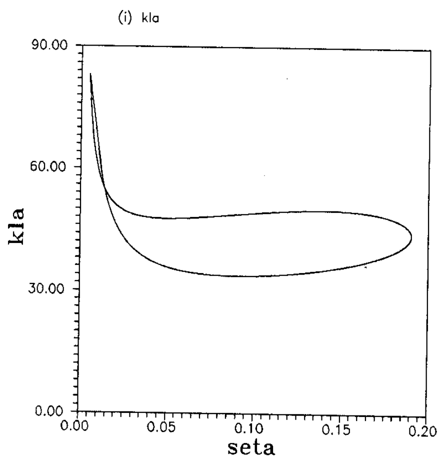
The continuity diagram (maximum specific maintenance rate Ki versus residence time θ) is shown in Fig. (3) and as the rest of model parameters shown in Table (1) will be studied in more details. The continuity diagram at different specific maintenance rate Ki will be discussed as far as the richness of the system is concerned. To have better understanding of the different bifurcation in the system. The diagram of Fig. (3) is divided into different regions according to the presence of HB points and LPs. And the static and dynamic bifurcation for each region are studied carefully. Different values of specific maintenance rate are chosen to study it at a different regions. Each will has its continuity diagram.

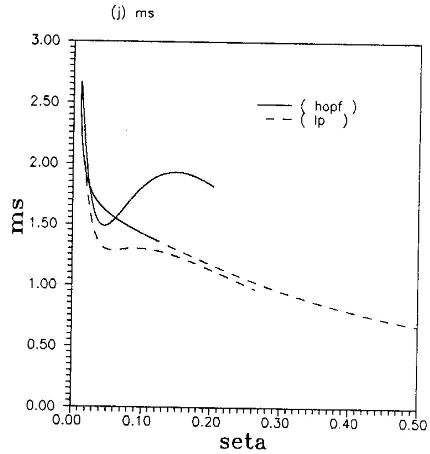
Figure (2) Two parameter continuation diagrams for some of the model parameters

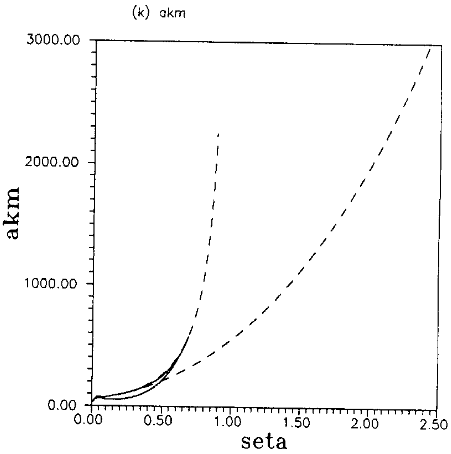



(g) kc
kc
seta
(hopf)
(lp)
0.00
2.00
4.00
6.00
8.00
0.00
0.10
0.20
0.30
0.40


(h) ki
ki
seta
(hopf)
(lp)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
0.00
0.10
0.20
0.30
0.40


(i) kla
kla
seta
0.00
30.00
60.00
90.00
0.00
0.05
0.10
0.15
0.20


(j) ms
ms
seta
(hopf)
(lp)
0.00
0.50
1.00
1.50
2.00
2.50
3.00
0.00
0.10
0.20
0.30
0.40
0.50


(k) akm
akm
seta
0.00
1000.00
2000.00
3000.00
0.00
0.50
1.00
1.50
2.00
2.50

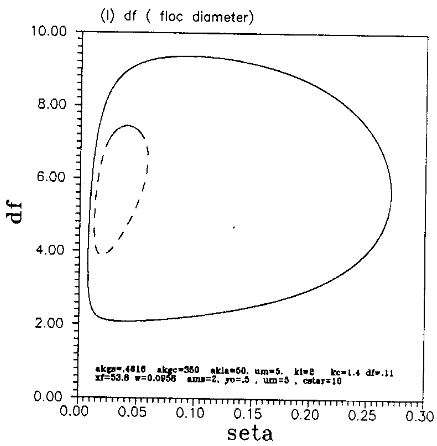
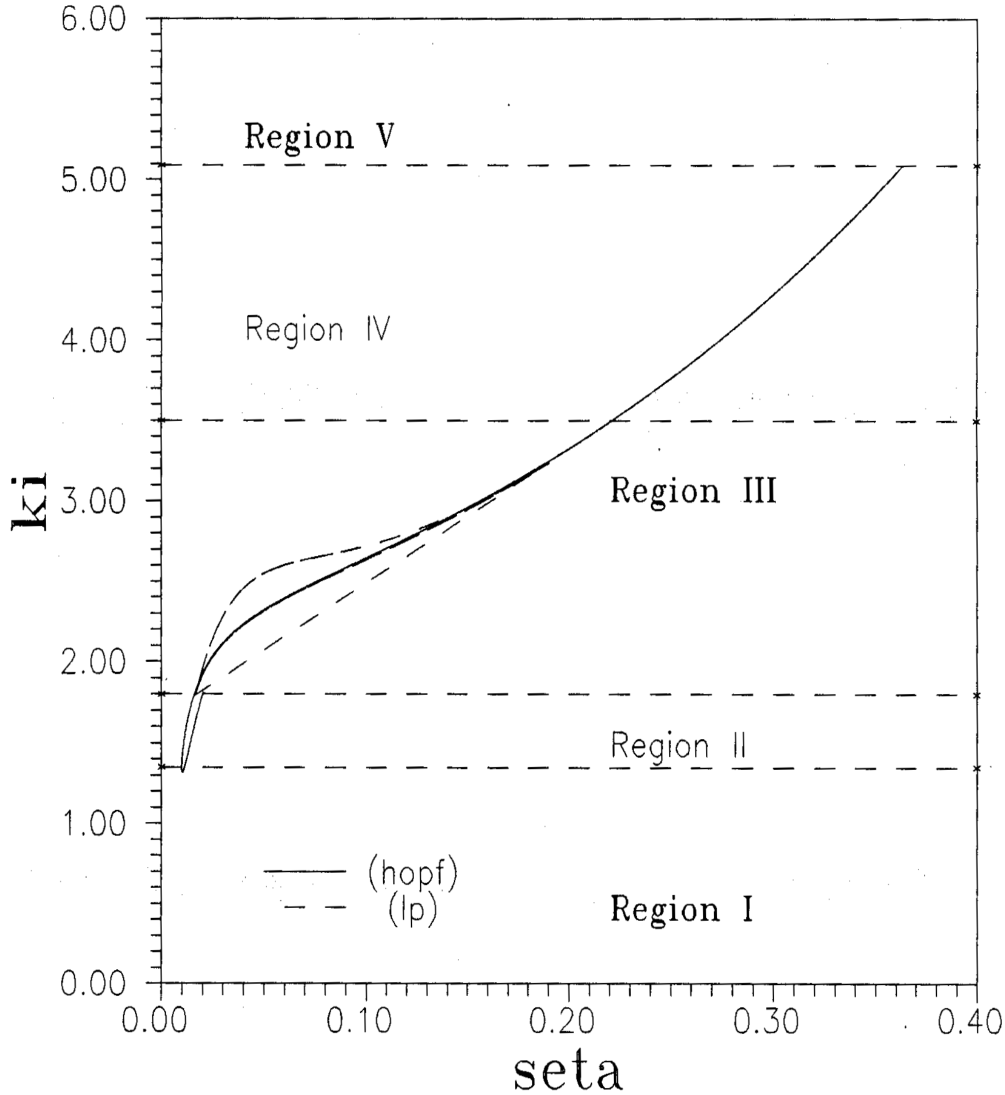

(l) df (floc diameter)
df
seta
akgs=.4616 akgc=350 akla=50. um=5. ki=2 kc=1.4 df=.11
xf=53.8 w=0.0958 ams=2. yo=.5 , um=5 , cstar=10
0.00
2.00
4.00
6.00
8.00
10.00
0.00
0.05
0.10
0.15
0.20
0.25
0.30

Fig (3) Regions of HB and LPs on maximum specific maintenance rate (ki) (two – parameter continuation)



Region (1) : Monod-Like Behavior

This region extends below the value of Ki that corresponds to the end of the LP curve at about Ki = 1.35. This region is characterized by the absence of any limit or Hopf Bifurcation points. A simple behavior is then extended in this region. Figure (4) shows the continuity diagram (specific maintenance rate Ki versus residence time θ), for example for Ki = 1.0. The continuation diagram shows one stable branch (solid line). It can be seen that starting from the initial value, the specific maintenance rate decrease. This unstructured models with classical Monod growth kinetics.

This behavior is also found from Ki = 4.9 (maximum value of HB curve) to the largest value of specific maintenance rate.

Region (2) : Hysteresis Behavior (in Presence of HB)

This region corresponds to value of Ki = 1.35 to Ki = 1.8 (where the HB curve makes a minimum value). This region is characterized by the presence of two HB points. The presence of HB means oscillations. But because the presence of the periodic solution between two static solutions, the system goes to any one of these static solutions and the periodic solution may not be reached at this region (actually, the domain of the periodic attractor is almost disappeared). The continuity diagram at Ki = 1.6 (for example) is shown in the Figure (7). The continuation diagram shows two stable branches (black lines) connected to unstable branch (dashed line). The solution is divided into three regions according to residence time's values as follows:

1. From 0 to .01266 h residence time (the first HB point) point attractor at low conversion steady state brach exists.
2. From 0.01722 h (the second HB point) to higher residence times the other point attractor at high conversion static branch exists.
3. Between two HB points bistability occurs between two point attractors.

Region (3) : Periodic and Non-Pperiodic Behavior

This region extends from Ki =1.8 to 3.5. It is characterized by the presence of more than one HB point and two LPs. This region can be divided as follows:

First Region:

This region is characterized by the presence of four HB points and two LPs. this region extends from Ki = 1.8 to Ki = 3.5 along the presence of the HB's curves with LP's curves together. A continuity diagram at Ki = 2.06 is constructed to study the behavior of this region.

As shown in Fig. (6) the solution is divided into five regions according to residence time's values as follows:

1- From 0h residence time to the first HB point at 0.0276 h, the static solution is the only one in this region.

2- Between the two HB points i.e. from 0.0276 h to 0.0361 h, there are bistability between two different static solutions. The domain of the attractor between these two static solutions has a periodic solution due to the presence of two HB. But because it is very narrow range the periodic solution could not be obtained.

3- From HB point at 0.0361 h to the next one at 0.0708 h, the static solution is the only one in this region.

Figure (4) Continuation Diagram at ki = 1.0

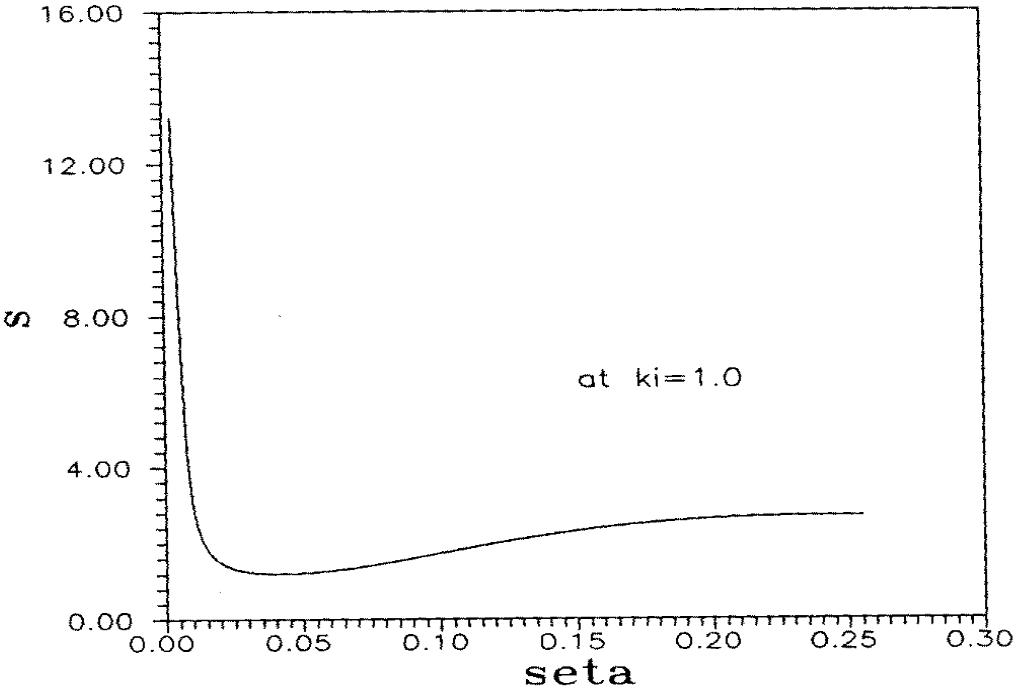
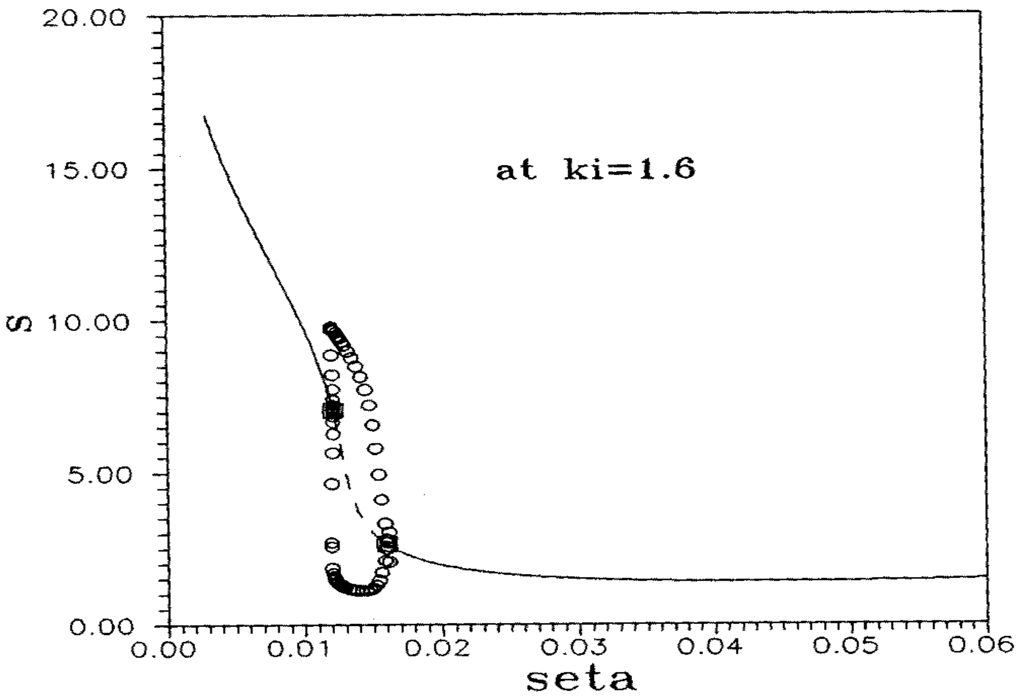


Figure (5) Continuation Diagram at ki=1.6



4- Between the two other HB points, i.e. from 0.0708 h to 0.221 h, the oscillations (periodic or non periodic) is the only solution along this wide range.
5- From the fourth HB point at 0.221 h to higher values of residence times, a unique static solution exists.

An important phenomenon in this region of stability (between two HB points i.e. from 0.0708 to 0.221) is that the operation under periodic solution is the only solution It covers a wide range of substrate concentration.

The presence of many kinds of attractors gives richness to the system. Such attractors are point attractors, periodic attractors and strange attractors (chaotic and/or non-chaotic attractors). Figure (7) gives the time trace and phase plane for the kinds of attractors exists for this range.

Second Region:
This region is characterized by the presence of two HB points and two LPS. This region extends from Ki = 2.15 to Ki = 3.2 (maximum value of LP curve). A continuity diagram at Ki = 2.15 is constructed to study the behavior of this region. the solution is divided into three regions according to residence times as follows:

1- From oh residence time to the first HB point at 0.0315h static solution exists.
2- From 0.255 h (the second HB point) to higher values of residence times, also static solution exists.
3- Between the two HB points, the stable periodic solution is the only one in this range. Figure (8) presents the continuity diagram at ki = 2.15.

Third Region :
This region is characterized by the presence of two HB points and absence of any LPs. This region extends from Ki = 3.2 (maximum value of LP curve) to Ki = 5.2. The presence of the HB's curve means oscillations occur.
A continuity diagram at Ki = 3.6, Fig. (9), is constructed to study the behavior of this region. The solution is divided into three regions according to residence time's values as follows:

1- From 0 h to the first HB point at 0.223 h, the steady state static solution exists.
2- From the second HB point at 0.41 h to the largest values of the residence time, another static solution also exists.
3- Between the two HB points, i.e. from 0.223 h to 0.41 h, the stable periodic solution of period one is the only one along this region.

Figure (6) Continuation diagram at ki=2.06

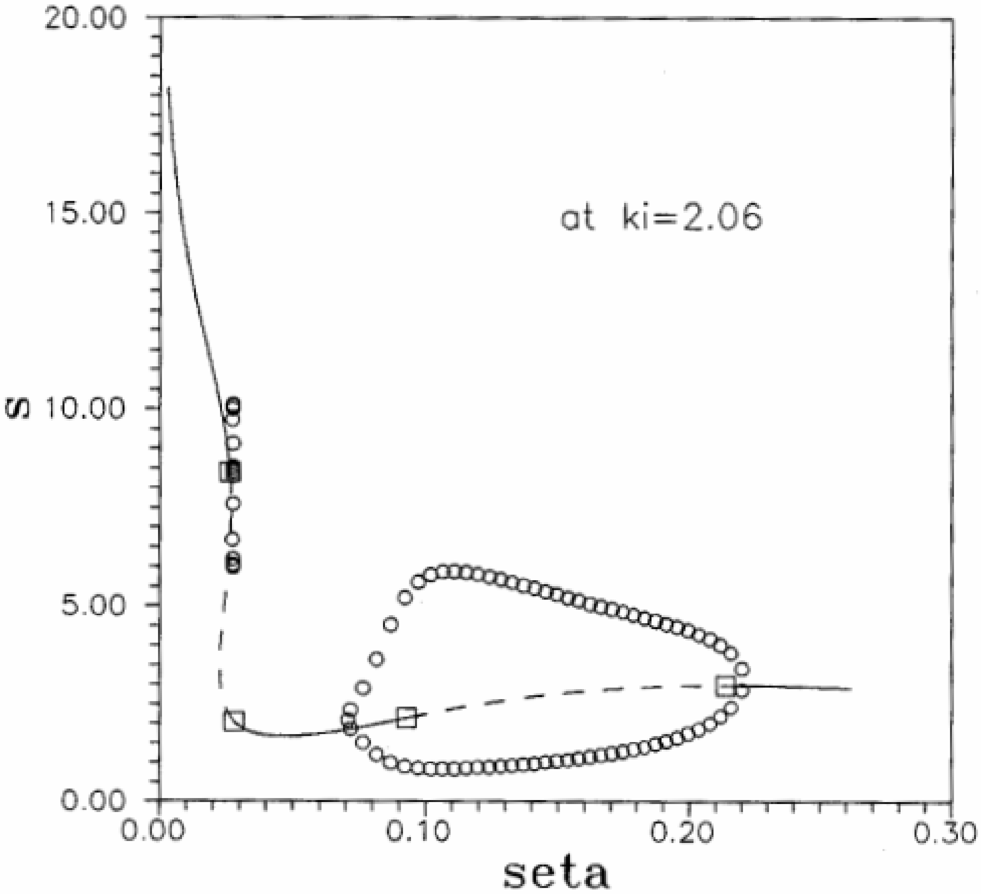


Fig (7) Time trace and phase plane for periodic and non periodic (chaotic) attractors for different values of seta

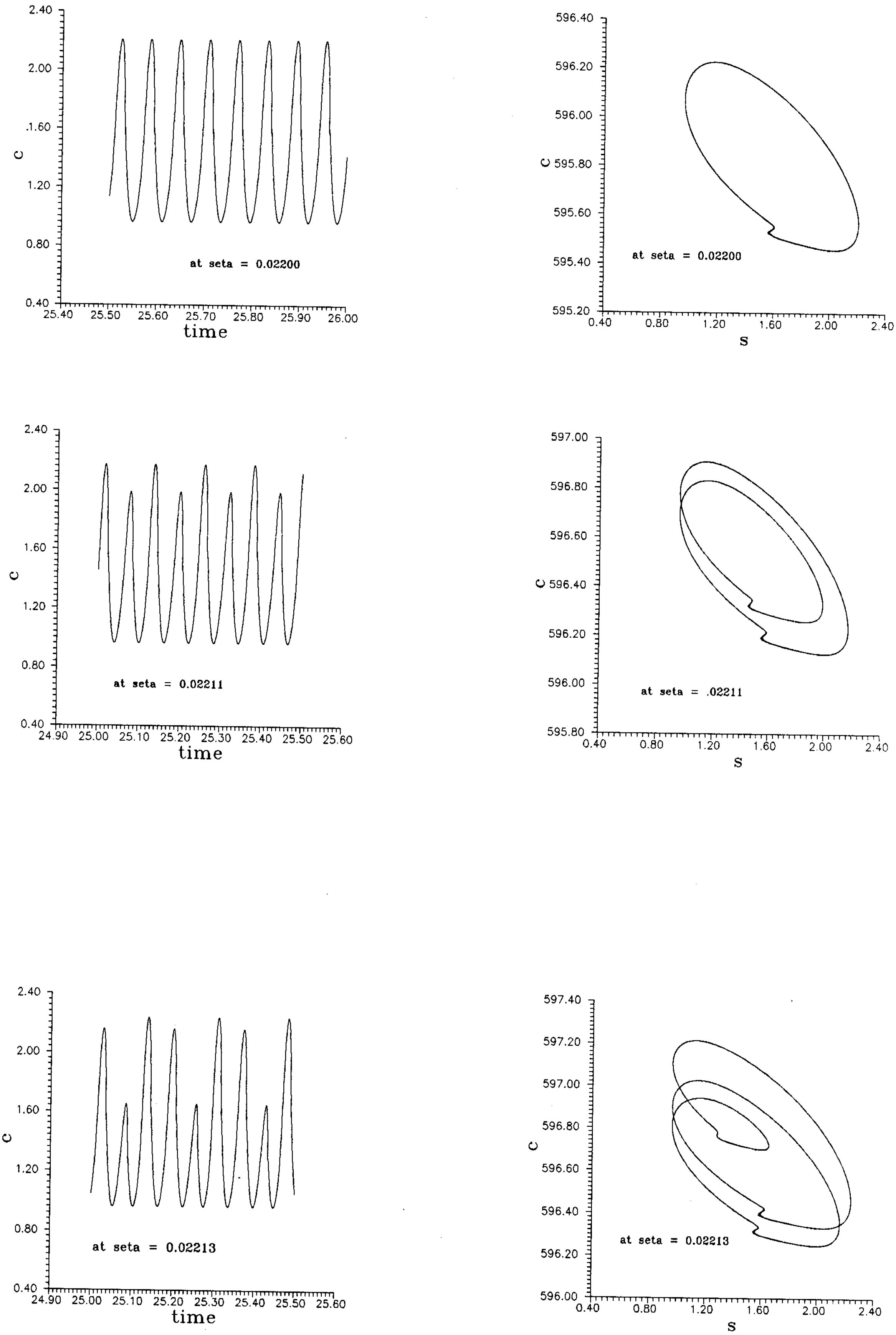
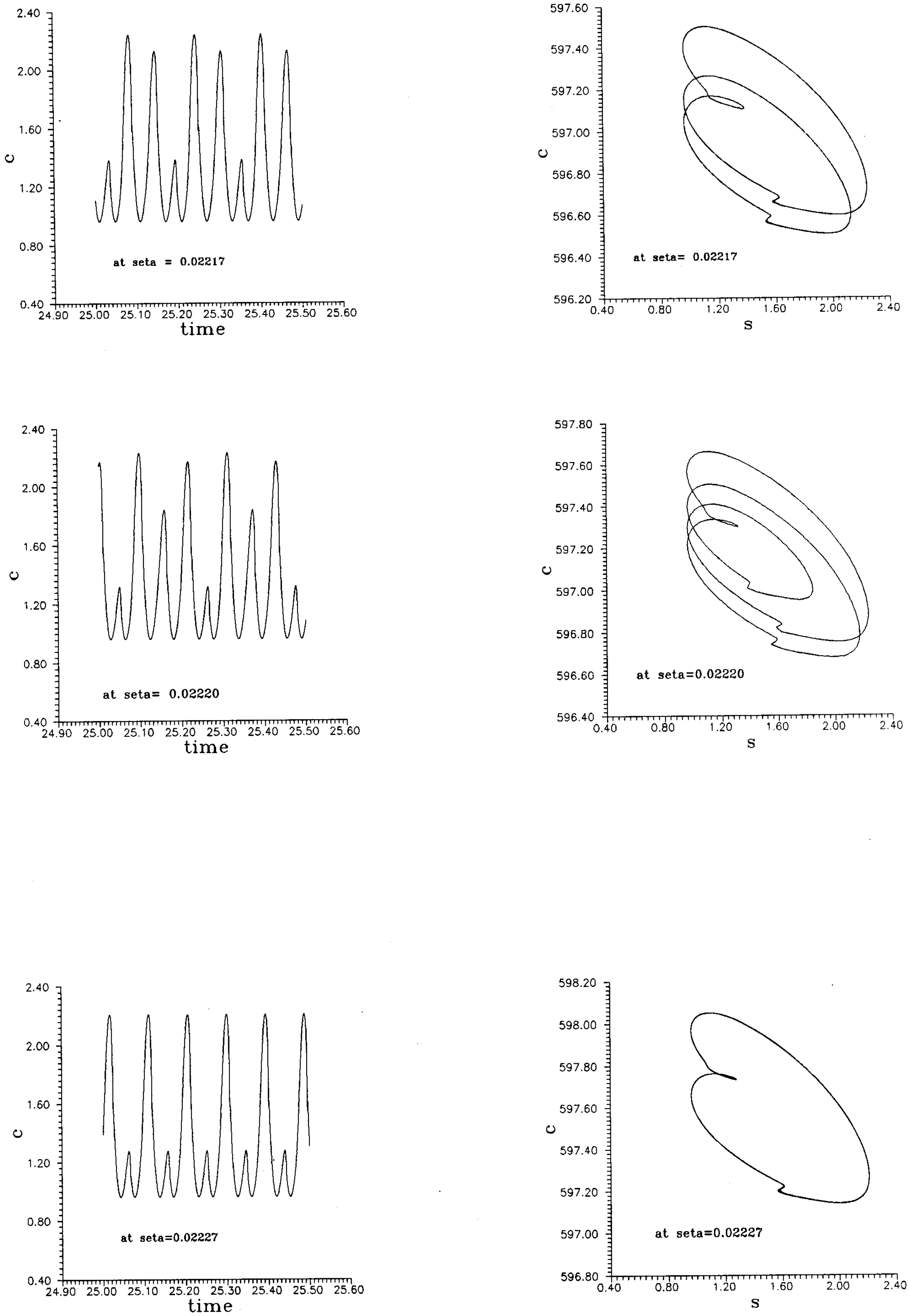


Fig (7) Time trace and phase plane for periodic and non periodic (chaotic) attractors for different values of seta



Fig(8) Continuation diagram at ki = 2.15

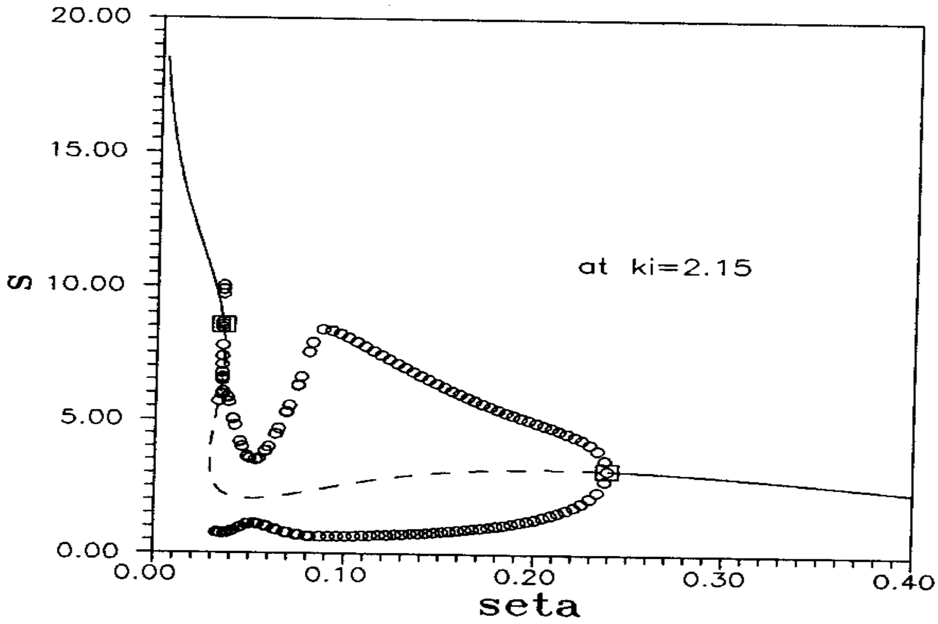
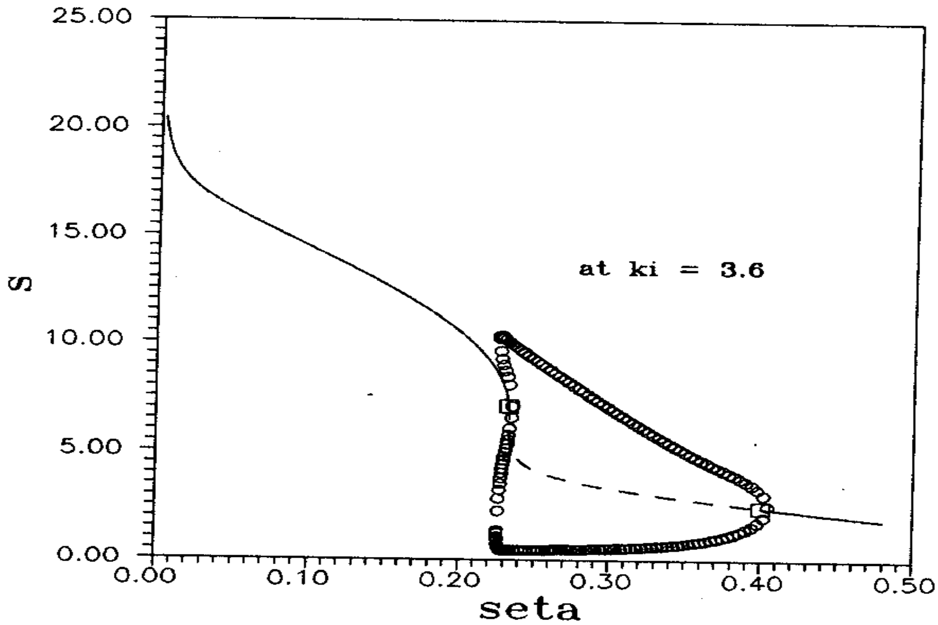


Figure (9) Continuation diagram at ki = 3.6



CONCLUSIONS

The investigation of the static and dynamic bifurcation of a bioreactor with cell ercycle based on a pseudo-homogenous floc model has revealed that the model is able to peridict oscillatory behavior for a wide range of model parameter. The analysis depicts a rich and complex variety of dynamic and steady state structures for the solution of the model. The model parameters illustrated in Table (1) are taken from realistic ranges given in literature.

Dynamic models were developed to undertake a qualitative study of this system. Detailed study was proposed at a different substrate feed concentrations to show the effect of residence time variation on output substrate concentration. Different kinds of solutions also exist. Point (steady state), periodic (with multi-periodicity) and chaotic attractors are found. In some cases periodic and chaotic solutions are the only solution exist for a wide range of substrate concentration where operation of the system must be carried to get the desired conversion.

Table (1) Model parameters

Parameter	Value
akgs (mass transfer coefficient of substrate)	0.4616
akgc (mass transfer coefficient of oxygen)	350
df (floc diameter)	0.11
um (maximum specific growth rate)	5
akc(equilibrium constant)	1.4
ams	2
Xf (biomass feed concentration)	53.8
w (purge factor)	0.0958
Sf (substrate feed concentration)	530
Akla (equilibrium constant)	50

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