Simulation of Substrate, Microbial Interaction with Recycle using MATLAB Computational Approach

C. P. Ukpaka, S. Orike, and F.U. Igwe

***Abstract*—This research outlines the microbial and substrate interaction in a plug flow bioreactor system for effective utilization of the substrate by the microorganism. To achieve this mathematical models were developed to monitor, predict and simulate the interaction characteristics of the bioreactor using the functional parameters for interaction of microbial and substrate concentration in a plug flow reactor system. The MATLAB computer program language was used to determine the interaction relationship between the substrate and microbial concentration upon the influence of bioreactor volume, space time and discharge time. The characteristics of the behavior in terms of decrease in substrate concentration with increase in microbial concentrate revealed the interaction in the bioreactor with recycle.**

***Index Terms*—Computational approach, MATLAB, Microbial, Recycle, Substrate**

I. Introduction

In microbial and substrate interaction processes in which enzyme-substrate complex disintegrate and products are produced by the activity of the cells mass in the substrate has yielded good result in either environmental clean-up in manufacturing process [1]. The process leads to the formation of useful products, as well as substance that are environmentally friendly such as the desired product biomass, heat and gases released [2]. The main concept of interaction is basically on the ability of the microbes to degradate the substrate without inhibiting influence from the environment [3]. In this case, when the bioreactor system is not inhibited, there is tendency of the high microbial and substrate interaction in process leading to absent of lag phase as well presence of acceleration and progressive phase and the utilization of the substrate will be at optimum [4]

When the stationary phase is achieved in the bioreactor and in this case substrate utilization remain constant [5]. Most of the products achieved during this processes are useful in beverages, remediation of polluted environment, drugs, alcohol production etc [6]. Investigation conducted on the usefulness of microorganism in enhancing national development has proved positive, indicating the great achievement in the world of science and technology.

In the microbial, substrate interaction, the metabolites of the primary and secondary products are formed as reviewed by various research groups [7]–[11]. Research conducted revealed that the significance of secondary concept of metabolites can be related or identified upon influence microorganisms' activities [12] as well as its hazardous characteristics in the system [13]. The recent investigation in the production of enzymes by the mechanisms of a bioreactor has shown a great advantage over other technologies that has been in practice for years [14].

In most processes of biochemical reactions for effective enzyme substrate complex formation the disintegration of it yields products that are environmental friendly and in most cases, the bioreactor is modified by the application of compounds that is added to the bioreactor to improve the fermentation process which order wise referred to as biotransformation [15]. Research conducted revealed the concept of microbial and substrate interaction as well as biomass increase in a favorable conditions and the transformation mechanism of raw materials by the application of microorganism [11]. It is revealed that the application of biotransformation can result to low energy level especially when nutrients added, acts as a rate limiting agent [16]. Microbial and substrate interactions are influenced by various components such as physicochemical properties of the process under investigation [17]. For effective controlling of a bioreactor, the following concepts must be put into consideration during the design for effective optimum of the characteristics of process [18]. The aim of the research is to ascertain the microbial and substrate interaction using MATLAB to monitor, predict and simulate the microbial and substrate utilization in a bioreactor.

II. Materials and Methods

The general material balance expression for microbial and substrate interaction is given in (1) as:

Material input + Formation by Biochemical reaction - Material output=Accumulation (1)

Material Balance in terms of Biomass (X)
Where the rate of reaction R=Velocity V, therefore the mathematical expression for each of functional parameter is expressed as:

$$\text{Input} = (F_O+F_R)X \quad (2)$$

$$\text{Output} = (F_O+F_R)(X+dX) \quad (3)$$

$$\text{Formation by Biochemical reaction} = R_X Dv \quad (4)$$

$$\text{Accumulation}=\frac{dX}{dt}V \quad (5)$$

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Substituting (2), (3), (4) and (5) into (1) we have:

$(F_O + F_R)X + R_X dV - (F_O + F_R)(X+dX) = (dX/dt)V$ (6)

Considering $dV = a_c dz$, as well as steady state (1) and rearranging we have:

$R_X a_c dz = (F_O+F_R)(dX)$ (7)

Considering the recycle ratio $R=\frac{FR}{Fo}$ therefore $F_R = RF_O$,

$R_X a_c dz = F_O(1+R)Dx$ (8)

Separating the variables of (8) as well integrating, we have:

$$\frac{\text{acdz}}{\text{Fo}(1+\text{R})} = \frac{dX}{Rx} \quad (9)$$

Integrating (9) using the following boundary conditions, thus:

At t = 0, Z = 0 to z, X = X_A to X_c

$$\frac{\text{ac}}{\text{Fo}(1+\text{R})}\int_0^Z dZ = \int_{XA}^{Xe}\frac{dX}{RX} \quad (10)$$

Similarly, for the Substrate, the form is also expressed as:

$$\frac{\text{ac}}{\text{Fo}(1+\text{R})}\int_0^Z dZ = \int_{SA}^{Se}\frac{ds}{Rs} \quad (11)$$

Taking a material balance for the substrate about the point of the mixing of the fresh feed and the recycle stream gives:

$S_oF_o + S_RF_R = (F_o + F_R)S_A$

$S_A = \frac{SoFo+SRFR}{Fo+FR}$

$S_A = \frac{SoFo+SRFoR}{Fo+FoR}$

$S_A = \frac{So+RSR}{1+R}$ (12)

Similarly, for the biomass, we have:

$X_oF_o + X_RF_R = (F_o + F_R)X_A$

$X_A = \frac{XoFo+XRFR}{Fo+FR}$

If $X_R = \Sigma Xe$

$X_A = \frac{XoFo+\Sigma XeFoR}{Fo+FoR}$

$X_A = \frac{Xo+\Sigma XeR}{1+R}$ (13)

Equations (12) and (13) define the boundary conditions on (11) and (10).

Recalling (11) we have:

$$\frac{\text{ac}}{\text{Fo}(1+\text{R})}\int_0^Z dZ = \int_{SA}^{Se}\frac{ds}{Rs}$$

Recall that for Monod's kinetics and Discharge Coefficient, the reaction rate with respect to the substrate Rs may be defined as:

$Rs = \frac{-UmSXa}{(Ks+S)Y}$

Substituting Rs into (11), we have:

$$\frac{\text{ac}}{\text{Fo}(1+\text{R})}\int_0^Z dZ = \int_{Se}^{SA}\frac{(Ks+S)Yds}{SXaUm}$$

$$\frac{\text{ac}}{\text{Fo}(1+\text{R})}\int_0^Z dZ = \frac{Y}{XaUm}\int_{Se}^{SA}\frac{(Ks+S)ds}{S}$$

$$\frac{\text{acXaUm}}{\text{Y Fo}(1+\text{R})}\int_0^Z dZ = \int_{Se}^{SA}\frac{Ksds}{S} + \int_{Se}^{SA} ds$$

Let $S_A = S_I$. Integrating the above equation gives:

$$\frac{\text{acXaUmZ}}{\text{Y Fo}(1+\text{R})} = \text{Ksln}\frac{Si}{Se} + (S_I - Se) \quad (14)$$

The definition of the Discharge Coefficient $Y = \frac{Xe-Xi}{Si-Se}$ can be used to derive an expression for the Biomass concentration by substituting $Y = \frac{Xe-Xi}{Si-Se}$ into (14).

$$\frac{\text{acXaUmZ(Si}-\text{Se)}}{\text{Fo}(1+\text{R})(\text{Xe}-\text{Xi})} = \text{Ksln}\frac{Si}{Se} + (S_I - Se)$$

$$\frac{\text{acXaUmZ(Si}-\text{Se)}}{\text{Fo}(1+\text{R})} = (\text{Xe} - \text{Xi})\text{Ksln}\frac{Si}{Se} + (S_I - Se)(\text{Xe} - \text{Xi})$$

$$\frac{\text{acXaUmZ}}{\text{Fo}(1+\text{R})} = \frac{Xe-Xi}{Si-Se}\text{Ksln}\frac{Si}{Se} + (\text{Xe} - \text{Xi})$$

$$\frac{\text{acXaUmZ}}{\text{Fo}(1+\text{R})} = \text{YKsln}\frac{Si}{Se} + (\text{Xe} - \text{Xi}) \quad (15)$$

Let us recall that for a given substrate concentration S, the rate of biodegradation is expressed thus:

$\frac{ds}{dt} = -\beta S$

On separation of variables for integration, the above equation gives:

$\int_{Si}^{Se}\frac{ds}{S} = -\int_0^t \beta dt$

Let $t = T$

$\ln\frac{Si}{Se} = \beta T$ (16)

Substituting (16) into (14) gives:

$$\frac{\text{acXaUmZ}}{\text{Y Fo}(1+\text{R})} = \text{Ks}\beta\text{T} + (S_I - Se)$$

Assuming $Xa = X_I$

$Se = (\frac{-\text{acXiUmZ}}{\text{Y Fo}(1+\text{R})} + S_I) + (\text{Ks}\beta)\text{T}$ (17)

Equation (17) is the Model equation for predicting the velocity (reaction rate) profile in terms of substrate concentration of a plug-flow fermenter.

Similarly, substituting (16) into (15) gives:

$$\frac{acXaUmZ}{Fo(1+R)} = YKs_{\beta}T + (Xe - Xi)$$

Assuming $Xa = X_I$

$$Xe = \left(\frac{acXiUmZ}{Fo(1+R)} + X_I\right) - (YKs_{\beta})T \qquad (18)$$

Equation (18) is the Model equation for predicting the velocity (reaction rate) profile in terms of biomass concentration of a plug-flow fermenter.

A. Computational Procedures

The developed mathematical model was monitored, predicted and simulated by chosen simulation parameters as presented using MATLAB. All the chosen parameters used for this investigation are useful and necessary to enables' we determine functional coefficients that control the microbial and substrate interaction in a bioreactor with recycling mechanism.

III. Results and Discussion

The results obtained from this investigation are presented in graph form with all computational parameters inputted in MATLAB as presented in the Figures shown below.

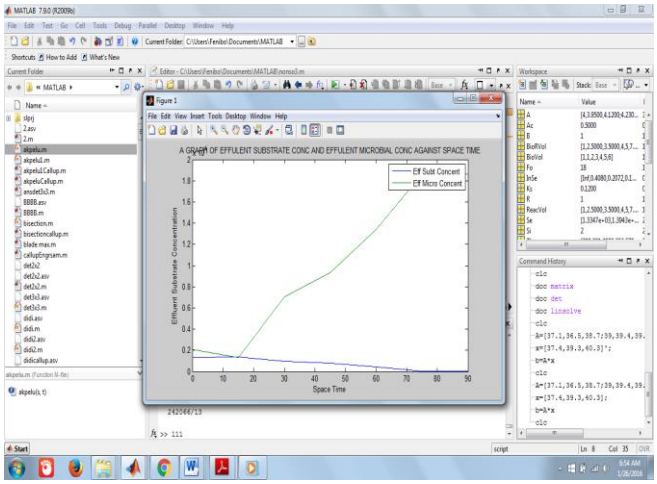

Fig.1. Effluent substrate concentration and effluent microbial concentration against space time

Fig.1 illustrates the interaction between the microbial and substrate in a bioreactor and result obtained shows increase in microbial concentration with decrease in substrate concentration with increase in space time. The variation in the microbial and substrate concentration can be attributed to the variation in the space time as well as other important factors that influence the bioreactor system.

The relationship between the effluent microbial concentration and the discharge time in the interaction of substrate and microbial concentration was investigated and result obtained revealed an increase in effluent microbial concentration with increase in discharge time as presented in Fig. 2. The variation in the effluent microbial concentration can be attributed to the variation in discharge time as well as functional parameters.

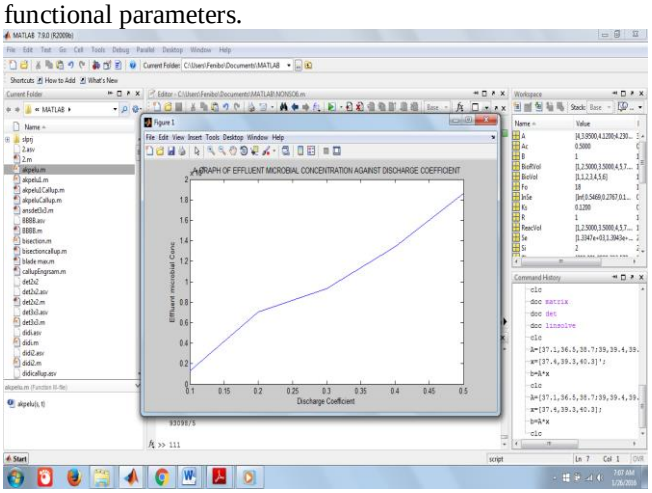

Fig. 2. Effluent microbial concentration against discharge time

Fig. 3 illustrates the characteristics of the effluent substrate concentration in a reactor volume and the results obtained revealed decrease in the effluent substrate concentration with increase in the reactor volume as monitored, predicted and simulated using MATLAB. The variation in the effluent substrate concentration can be attributed to the variation in the reactor volume as well as the functional parameters and coefficients. Similarly, it is seen from Fig. 4 that the substrate concentration decreases with increase in the bioreactor volume. The variation in the substrate concentration can be attributed to the variation in the bioreactor volume.

Fig. 5 illustrates the relationship between the effluent microbial concentration and reactor volume as well as increase in effluent microbial concentration was observed with increase in reactor volume. The variation in the effluent microbial concentration can be attributed to the variation in the reactor volume. Similarly, as presented in Fig. 6 it is seen that increase in microbial concentration was observed with increase in bioreactor.

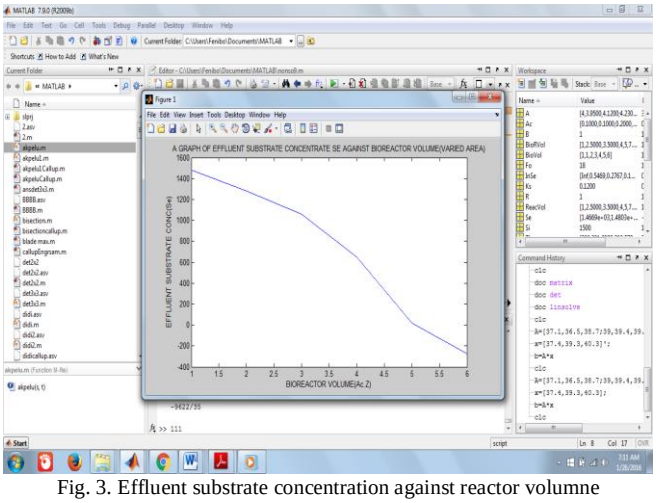

Fig. 3. Effluent substrate concentration against reactor volumne

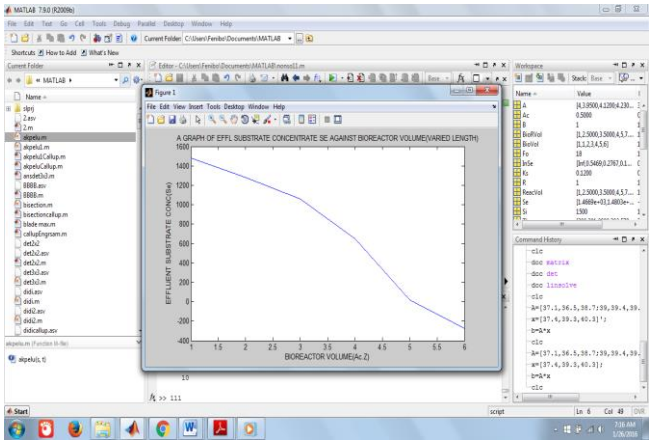

Fig. 4. Substrate concentration against bioreactor volume

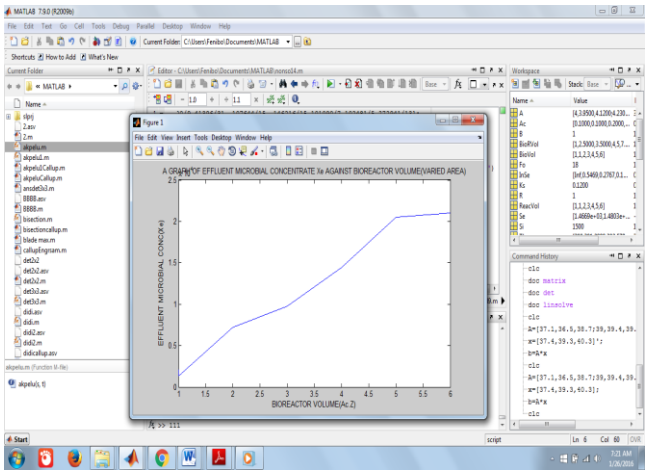

Fig. 5. Effluent microbial concentration against bioreactor volume

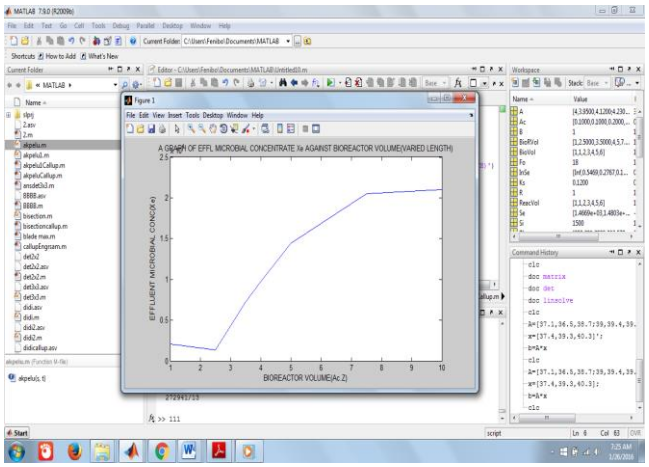

Fig. 6. Effluent microbial concentration against bioreactor volume

From the result obtained from the graph above, the substrate concentration across time increases while the microbial concentration decreases. As the reaction occur across different time interval, the substrate concentration tends towards maximum while the microbial concentration reduces to an insignificant level, thereby leading to an end in the reaction process.

It is also noted that, across the reactor volume, the substrate concentration decreases across the volume of the bioreactor, while the microbial concentration increases across the reactor volume.

IV. Conclusion

Research conducted reveals the following observations:

1. It is observed that the volume of the reactor, the time of the reaction, the space velocity, discharge coefficients are variables that determines the nature and rate of the substrate and microbial concentration in a bioreactor.
2. The model equations to check their profile (substrate and microbial) has been developed and solved in this research work using MATLAB as the run out results are presented in the appendix.
3. Increase in microbial concentration without inhibitor yielded decrease in substrate concentration
4. MATLAB is a useful tool for monitoring, predicting and simulating the relationship between microbial and substrate utilization in a bioreactors system.

Appendix

The following are parameters used to simulate the graphs shown in Figs. 1-6 using MATLAB.

For Fig. 1:

```
% Modelling Of the Velocity Profile Of A Bioreactor with Recycle:
 Fo=18;%l/hr
Um=0.25;%1/hr
Ks=0.12;
Y=0.42;
R=1;
Z=10;
Ac=0.5;%m2
B=1;%1/hr
for Si=[2000,1900,1800,1700,1650,1600,1500];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=[0:15:90];% SpaceTime
Se=(Si-((Ac*Z*Xi*Um)/(Y*Fo*(1+R))))+(Ks*B).*V;
end
format rat
disp(Se)
OUTPUT: Columns 1 through 6
  42709/32      68322/49      61193/65      12943/17      12109/28
439/21
Column 7
  2384/105
Fo=18;%l/hr
Um=0.25;%1/hr
Ks=0.12;
Y=0.42;
R=1;
Z=10;
Ac=0.5;%m2
B=1;%1/hr
for Si=[100,100,80,50,15,5,2];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=[0:15:90];
Xe=(Xi+((Ac*Z*Xi*Um)/(Fo*(1+R))))-(Y*Ks*B).*V;
end
format rat
disp(Xe)
Columns 1 through 6
  18625/9       63186/47      35173/5       121033/13     147932/11
167591/9
 Column 7
 242066/13
Se=[42709/32,68322/49 , 61193/65,12943/17,12109/28,439/21,2384/105  ]
;
Xe=[ 18625/9,63186/47,35173/5 ,121033/13,147932/11,167591/9
,242066/13  ];
V=[0:15:90];
plot(V,Se,V,Xe)
xlabel('Space Time')
ylabel('Effluent Substrate Concentration')
```

```
title('A GRAPH OF EFFULENT SUBSTRATE CONC AND EFFULENT MICROBIAL CONC AGAINST SPACE TIME')
legend('Eff Subt Concent','Eff Micro Concent')
```

For Fig. 2:

```
Ac=0.5;%m2
B=1;%1/hr
for Si=[2000,1900,1800,1700,1650,1600,1500];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=0:15:90;
p=1./Si;
q=(Y*Fo*(1+R));
r=(Ac*Z.*Xi*Um);
s=1/(Ks*B);
t=1./V;
InSe=(p-(q./r))+s.*t;
end
format rat
disp(InSe)
OUTPUT:Columns 1 through 6
  1/0        2005/3666       843/3047       343/1859       365/2633
2315/20836
  Column 7
  321/3467
Fo=18;%l/hr
Um=0.25;%1/hr
Ks=0.12;
R=1;
Z=10;
Ac=0.5;%m2
B=1;%1/hr
for Si=[100,100,80,50,15,5,2];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=[0:15:90];
Y=[0.1,0.1,0.2,0.3,0.4,0.5,0.5];
r=1/Ks*B;
Xe=(Xi+(Ac*Z*Xi*Um)/(Fo*(1+R)))-(Ks*B*V).*Y;
end
format rat
disp(Xe)
OUTPUT:Columns 1 through 6
  18625/9        32279/24       161814/23       74487/8        26897/2
37241/2
  Column 7
 93098/5
Y=[0.1,0.1,0.2,0.3,0.4,0.5,0.5];
Xe=[ 18625/9,32279/24,161814/23,74487/8,26897/2 ,37241/2,93098/5  ];
plot(Y,Xe)
xlabel('Discharge Coefficient')
ylabel('Effluent microbial Conc')
title('A GRAPH OF EFFLUENT MICROBIAL CONCENTRATION AGAINST DISCHARGE COEFFICIENT')
```

For Fig. 3:

```
Fo=18;%l/hr
Um=0.25;%1/hr
Ks=0.12;%g/h
Y=0.42;
R=1;
Z=10;%m
B=1;%1/hr
for  Si=[2000,1900,1800,1700,1650,1600,1500];
    Ac=[0.1,0.1,0.2,0.3,0.4,0.5,0.6];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=[0:15:90];
Se=(Si+(Ks*B.*V))-((Xi*Um)/(Y*Fo*(1+R))).*Ac*Z;
end
format rat
disp(Se)
OUTPUT:Columns 1 through 6
   42541/29       53291/36       19181/15       37064/35       11006/17
439/21
  Column 7
  -9622/35
%Bio Reactor Vol
Z=10;
 Ac=[0.1,0.1,0.2,0.3,0.4,0.5,0.6];
 biovol=Z.*Ac;
disp(biovol)
OUTPUT: Columns 1 through 6
 1   1       2       3       4       5
 Column 7, 6
%A GRAPH OF EFFLUENT SUBSTRATE CONCENTRATE SE AGAINST BIOREACTOR VOLUME
BioVol=[ 1,1,2,3,4,5,6 ];
Se=[42541/29,53291/36,19181/15,37064/35,11006/17, 439/21, -9622/35]
plot(BioVol,Se)
xlabel('BIOREACTOR VOLUME(Ac.Z)')
ylabel('EFFLUENT SUBSTRATE CONC(Se)')
title('A GRAPH OF EFFLUENT SUBSTRATE CONCENTRATE SE AGAINST BIOREACTOR VOLUME(VARIED AREA)')
```

For Fig. 4:

```
%Bio Reactor Vol GRAPH 7
 Ac=0.5;
 Z=[2,5,7,8,10,15,20];
 biovol=Ac.*Z;
disp(biovol)
OUTPUT:Columns 1 through 6
    1      5/2      7/2       4        5       15/2
 Column 7,  10
BioRVol=[ 1,5/2,7/2,4,5,15/2,10];
Se=[42541/29,53291/36,19181/15,37064/35,11006/17,439/21,-9622/35];
plot(BioVol,Se)
xlabel('BIOREACTOR VOLUME(Ac.Z)')
ylabel('EFFLUENT SUBSTRATE CONC(Se)')
title('A GRAPH OF EFFL SUBSTRATE CONCENTRATE SE AGAINST BIOREACTOR VOLUME(VARIED LENGTH)')
```

For Fig. 5:

```
Fo=18;%l/hr
Um=0.25;%1/hr
Ks=0.12;%g/h
Y=0.42;
R=1;
Z=10;%m
B=1;%1/hr
for Si=[2000,1900,1800,1700,1650,1600,1500];
   Ac=[0.1,0.1,0.2,0.3,0.4,0.5,0.6];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=[0:15:90];
Xe=(Xi-Y*Ks*B.*V)+((Xi*Um)/Fo*(1+R)).*Ac*Z;
end
format rat
disp(Xe)
OUTPUT:Columns 1 through 6
18500/9       41396/31       107644/15      146216/15      101090/7
102481/5
Column 7
272941/13
Xe=[18500/9,41396/31 ,107644/15
,146216/15,101090/7,102481/5,272941/13];
ReacVol=[1,1,2,3,4,5,6 ];
plot(ReacVol,Xe)
xlabel('BIOREACTOR VOLUME(Ac.Z)')
ylabel('EFFLUENT MICROBIAL CONC(Xe)')
title('A GRAPH OF EFFLUENT MICROBIAL CONCENTRATE Xe AGAINST BIOREACTOR VOLUME(VARIED AREA)')
```

For Fig. 6:

```
Fo=18;%l/hr
Um=0.25;%1/hr
Ks=0.12;%g/h
Y=0.42;
R=1;
Z=10;%m
B=1;%1/hr
for Si=[2000,1900,1800,1700,1650,1600,1500];
   Ac=[0.1,0.1,0.2,0.3,0.4,0.5,0.6];
Xi=[2000,1300,6800,9000,13000,18000,18000];
V=[0:15:90];
Xe=(Xi-Y*Ks*B.*V)+((Xi*Um)/Fo*(1+R)).*Ac*Z;
end
format rat
disp(Xe)
```

```
OUTPUT:Columns 1 through 6
18500/9       41396/31      107644/15      146216/15
101090/7      102481/5
 Column 7
272941/13
Vol=[  1,5/2 ,7/2,4 ,5,15/2,10 ];
  Xe=[18500/9 ,41396/31,107644/15,146216/15
,101090/7,102481/5, 272941/13];
plot(Vol,Xe)
xlabel('BIOREACTOR VOLUME(Ac.Z)')
ylabel('EFFLUENT MICROBIAL CONC(Xe)')
title('A GRAPH OF EFFL MICROBIAL CONCENTRATE
Xe AGAINST BIOREACTOR VOLUME(VARIED
LENGTH)')
```

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