

# 20BTC602J-BIOPROCESS MODELLING AND SIMULATION LABORATORY

*Offered to*

**M.Tech – Biotechnology**

**II Semester**



# SRM

INSTITUTE OF SCIENCE & TECHNOLOGY  
(Deemed to be University u/s 3 of UGC Act, 1956)

**Department of Biotechnology**  
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## Syllabus cum Index

Ex.NO	Name of the Experiment	Page.No
1	PARAMETERS ESTIMATION IN ADSORPTION KINETICS USING CURVE FITTING TOOL IN MATLAB	
2	ESTIMATION OF BACTERIAL GROWTH KINETIC PARAMETER USING CURVE FITTING TOOL IN MATLAB	
3	MODELING OF BATCH CULTURE USING MATLAB	
4	MODELING IN FED BATCH CULTURE IN MATLAB	
5	MODELING IN CONTINUOUS CULTURE USING MATLAB	
6	MODELING IN PRODUCT FORMATION USING MATLAB	
7	MODELLING OF BATCH CULTURE BY BERKELEY-MADONNA	
8	MODELLING OF CONTINUOUS CULTURE BY BERKELEY-MADONNA	
9	MODELLING OF FED BATCH CULTURE BY BERKELEY-MADONNA	
10	SIMULATION BY SIMULINK IN BATCH CULTURE	
11	SIMULATION BY SIMULINK IN CONTINUOUS CULTURE	
12	SIMULATION BY SIMULINK IN FED BATCH CULTURE	
13	SOLVING MATERIAL BALANCE USING SUPERPRO DESIGN	

**EXP NO: 1**

**DATE:**

**PARAMETERS ESTIMATION IN ADSORPTION KINETICS USING CURVE FITTING  
TOOL IN MATLAB**

**AIM:**

To estimate the parameters in adsorption kinetics using curve fitting tool in MATLAB.

**THEORY:**

MATLAB is both computer programming language and software environment for using that language effectively. MATLAB is a powerful general purpose system or environment for doing mathematics, scientific and engineering. In MATLAB, curve fitting tool box provides an application and functions for fitting curves and surfaces to data. The tool box exploratory data analysis, pre-process and post-process data, compare template models and remove outliers. The library provide optimized solver parameter and starting conditions to improve the quality of your fits.

Adsorption is the adhesion of atoms, ions or molecules from a gas, liquid or dissolved solid to a surface. In this experiment the effect of initial dye concentration were used to test the different adsorption isotherm models to know the adsorption mechanism. The adsorption isotherm plays an important role in the determination of the maximum adsorption capacity of the adsorbent. To adapt to the considered system, the isotherms of Langmuir, Freundlich, Redlich-Peterson and Temkin have been considered.

**The Langmuir Isotherm**

The non-linear equation for the Langmuir isotherm model is expressed as follows:

$$q_e = \frac{q_m K_L C_e}{1 + K_L C_e}$$

where  $C_e$  is the dye concentration at the equilibrium state of the system (mg/L),  $q_m$  (mg/g) and  $K_L$  (L/mg) are the Langmuir constants, representing the maximum adsorption capacity for the solid phase loading, and the energy constant related to the heat of adsorption, respectively.

**The Freundlich Isotherm**

The Freundlich isotherm model is a well known relationship describing the adsorption process. This isotherm is an empirical equation which can be expressed as follows:

$$q_e = K_f C_e^{1/n}$$

where  $K_f$  is the Freundlich constant  $((\text{mg/g})(\text{L/mg})^{1/n})$  related to the bonding energy.  $K_f$  can be defined as the adsorption or distribution coefficient, and it represents the quantity of the dye adsorbed for unit equilibrium concentration.  $1/n$  is the heterogeneity factor, and  $n$  is the gauge of the deviation from the linearity of adsorption. Its value indicates the degree of non-linearity between the solution concentration and adsorption as follows: if  $n=1$ , the adsorption is linear; if  $n<1$ , it implies that the adsorption process is favoured by chemisorption and if  $n>1$ , the adsorption process is favoured by physisorption.

### The Redlich-Peterson Isotherm

The Redlich-Peterson isotherm is a combination of the Langmuir- Freundlich model. The equation is given as:

$$q_e = \frac{K_R C_e}{1 + \alpha_R C_e^\beta}$$

where  $K_R$  is the Redlich-Peterson isotherm constant (L/g),  $\alpha_R$  is the Redlich-Peterson isotherm constant (L/mg), and  $\beta$  is the exponent which lies between 0 and 1. The constant  $\beta$  can characterize the isotherm; if  $\beta=1$ , the Langmuir will be the preferable isotherm, while if  $\beta=0$ , the Freundlich isotherm will be the preferable isotherm.

### The Temkin Isotherm

The Temkin isotherm model takes into account the adsorbent-adsorbate interactions. This model assumes the following: the heat of adsorption of all the molecules in the stratum decreases linearly with treatment due to adsorbent-adsorbate interactions, and the adsorption is characterized by a uniform allocation of binding energies, up to a maximum binding energy. The Temkin isotherm has been applied in the following form:

$$q_e = B \ln(AC_e)$$

where  $A$  and  $B$  are Temkin isotherm constants.

## PROCEDURE

1. Prepare the stock solution using 100 ppm of RB-5 dye.
2. Make the dilutions i.e. 20,40,60,80,100 ppm.
3. Take the O.D at 595 nm.
4. Then, about 50 mg of adsorbent was added in the solution.

- Kept it in the shaker for 24 hours. Take the OD at 595 nm.

### Curve Fitting In Matlab

- Enter the x (Ce) value and y(qe) value
- Go to start in MATLAB and select toolbox → curve fitting → cftool.
  - Feed x Langmuir:  $f(x) = (q \cdot k \cdot x) / (1 + k \cdot x)$
  - Frendlich:  $f(x) = k \cdot x^{(1/n)}$
  - Redlich Peterson:  $f(x) = (k \cdot n) / (1 + a \cdot x^b)$
  - Temkin Isotherm:  $f(x) = b \cdot \log(a \cdot x)$
- and y data i.e.
 

x data =x

y data =y
- Enter data set name y vs x.
- Create the data set
- Fit name and type of fit (custom equation)
- Select new and write the general equation for the respective adsorption isotherms.
- Interpret the results and compare the adsorption isotherms.

### Observation:

Co(initial dye conc mg/L.)	Initial OD (at 595nm)	Final OD (at 595nm)	Ce (x)	M(g)	qe=(Co-Ce/M)
20					
40					
60					
80					
100					

### Standard curve plot:

Ppm	Absorbance@ 595 nm
5	
10	
15	
20	
25	

**OBSERVATION:**

**RESULT:**

**EXP NO: 2**

**DATE:**

**ESTIMATION OF BACTERIAL GROWTH KINETIC PARAMETER USING CURVE  
FITTING TOOL IN MATLAB**

**Aim:**

To study whether the bacterial growth kinetic parameters are affected by RBBR dye

**Theory:**

Theory explains the modelling of growth kinetics using bacterial consortium in the presence of RemazolBrilliant Blue R (RBBR) dye. The dye acts as a C source for the growth of microorganisms. The utilization of dye leads to the formation of biomass. As the dye decolouration is the result of the microbial activity, the kinetics of contaminant degradation is closely related to the kinetics of microbial growth. The obtained biomass concentrations and substrate concentration at different time intervals for various initial concentrations of dye was used to calculate specific growth rate and given by Eq.1.

$$\mu = \frac{1}{x} \frac{dx}{dt} \dots\dots\dots (1)$$

where,  $\mu$  is the specific growth rate ( $h^{-1}$ ),  $x$  is the biomass concentration ( $g\ l^{-1}$ ) at time  $t$  (h), and  $dt$  is change in time (h) for the change in biomass concentration,  $dx$ . After integration, Eq.1 can be represented by Eq.2:

$$\ln x = \ln x_0 + \mu t \dots\dots\dots(2)$$

where,  $x_0$  is the initial biomass concentration ( $g\ l^{-1}$ ) at  $t = 0$ . A linear least square method was used to calculate the specific growth rate using the data obtained for log phase at different initial concentration of dye. A plot of  $\ln x$  versus  $t$  gives a straight line with  $\ln x_0$  as its intercept and  $\mu$  as the slope. The lag phase and death phase data are not considered for the estimation of specific growth rate. The step size for  $\ln x$  and  $t$  used to calculate specific growth rate in linear least square method at different initial dye concentrations.

**Monod model:**

Monod model relate the specific growth rate to the concentration of a single growth-controlling substrate (S) via two parameters, the maximum specific growth rate ( $\mu_{max}$ ) and the substrate affinity constant ( $K_s$ ) as given by :

$$\mu = \mu_m \frac{S}{K_s + S} \dots\dots\dots(3)$$

Eq. 3 has two unknown parameters ( $\mu_m$  and  $K_s$ ), which was linearized as given by Eq. 4 and was solved using the method of linear least squares.

$$\frac{1}{\mu} = \frac{K_s}{\mu_m} \left(\frac{1}{S}\right) + \left(\frac{1}{\mu_m}\right) \dots\dots\dots(4)$$

The graph was plotted between  $(1/\mu)$  and  $(1/S)$  by which the intercept of the line gave the value of  $\mu_m$  and the slope gave  $K_s$ .

Monod model is a simple model. But the model only describes the dependence of biodegradation rate on the biomass concentration. The limitation of classical Monod's equation is that it does not account for the fact that cells may need substrate or may synthesize product even when they do not grow. The original Monod equation was modified by Powell which takes into account of some of the limitation of Monod model.

**Powell's model:**

Monod equation was modified by introducing the terms of maintenance, expressed as the threshold substrate concentration ( $S_{min}$ ) and maintenance rate ( $m$ ). This led to the modified Monod model which may be due to the incorporation of maintenance rate in Powell model.

$$\mu = (\mu_{max} + m) \frac{S}{K_s + S} - m \dots\dots\dots(5)$$

**Haldane model:**

Haldane model was originally proposed for substrate inhibition in 1968. According to Haldane model, the specific growth rate can be represented by

$$\mu = \frac{\mu_{max} S}{K_s + S + \left(\frac{S^2}{K_I}\right)} \dots\dots\dots(6)$$

where,  $K_I$  is the substrate inhibition constant ( $mg\ l^{-1}$ ).

**Luong model:**

The inhibitory effect of substrate on biomass growth under batch conditions can be represented by a mathematical expression which was proposed by Luong (1987). This model is based on certain assumptions which include no lag phase, organism death, endogenous respiration, substrate used for maintenance energy, or inhibition by products. The model incorporates a term given as  $S_m$  ( $mg\ l^{-1}$ ) critical inhibitor concentration above which the growth is completely inhibited.

$$\mu = \frac{\mu_m S}{K_s + S} \left(1 - \frac{S}{S_m}\right)^n \dots\dots\dots(7)$$



where  $S_m$  ( $\text{mg l}^{-1}$ ) is the critical inhibitor concentration above which biodegradation stops,  $n$  is the positive integer in the Luong model.

**Edward model:**

Edwards discussed various reasons for the substrate inhibition which affects the microbial growth. The reasons for substrate inhibition could be the formation of intermediates, or products; changed activity of one or more enzymes; dissociation of one or more enzymes or formation of metabolic aggregates.

**Procedure:**

1. Prepare 600ml of LB medium
2. Transfer 100ml of medium in six conical flasks labelled as C1, C2, S1, S2, S3, S4
3. Take 1ml of sample from each conical flask and measure absorbance at 610nm.
4. C1 is control1 which contains only medium and C2 is the control 2 which corresponds to 0 ppm, containing medium and 10ml of bacterial consortium.
5. S1, S2, S3 and S4 vary in concentration from 5, 15, 30 and 50 ppm of RBBR dye.
6. Inoculate 10ml of bacterial consortium to all flasks except C1 and C2.
7. Measure the OD at 610 and 595 nm respectively in order to obtain the substrate consumption and dye utilization.
8. Substrate consumption is measured by DNS method.
9. Repeat the procedure for 3 days on a time interval of 5 hrs.
10. Results obtained were fitted into the growth models using MATLAB software.

**Observation:**

Substrate (ppm) (x)	Biomass		$\mu(\text{hr}^{-1})$ (y)
	0 hr	16 hr	

**Result:**

**EXP NO: 3**

**DATE:**

**MODELING OF BATCH CULTURE USING MATLAB**

**AIM:**

To model microbial batch growth kinetics in MATLAB.

**Theory**

**Basic definition and scope of Model –**

Description of reality is basically termed as “Model”. For example maps of the city describing the locations of roads, parks colonies could also be described as model as they are the pictorial representation of the reality. Similarly graphs indicating population growth in a country in different years also gives an elegant presentation of facts about the population and therefore be called as model representation of population statistics. The extrapolation of the above definition(s) could also lead to the conclusion that mathematical model is nothing but the kinetic description of substrate disappearance primarily leading to appearance of growth and product by cellular (microorganism, plant or animal cell) activity in the bioreactor. Cell cultivations are done under aseptic conditions in bioreactor to produce strategic metabolites which have commercial values. However this is a labor intensive process thereby normal process optimization procedure for optimization of process parameters &/or culture mode(s) becomes a very tedious and frustrating exercise. On the contrary development of a mathematical model not only facilitates easy understanding of culture behavior under different cultivation conditions but also helps in the design of suitable reactor optimization strategy(ies) for maximum yield and productivity of a particular metabolites. This approach is

particularly important for plant cell cultivation for the production of valuable secondary metabolites which exhibit slower growth with the result even a single batch cultivation takes months to complete.

#### **Unstructured Mathematical model and its limitation –**

Accurate description of cell activity in model is very important for realistic description of culture behavior. Usually unstructured models are used as their experimental validation is simple and are easy to use for the prediction of reactor operation strategies. These models however assume cell to be described by a single number i.e., biomass which is easy measurable but it does not make any distinction between living and/or dead cells. This rather simplistic assumption of biomass as a representation of cell activity substitutes usage of thousands of highly complex reactions rate equations which are typically involved in the growth process, thereby it provides easy solution of the model equations but it invariably fails to describe the dynamic behavior of cells particular when the model is extrapolated to describe the cultivations other than what were used for identification of its model parameters. The typical situations where the unstructured model invariably fails are description of lag phase, fed batch cultivations & transients (shift up and shift down in dilution rates) in continuous cultivations where the culture metabolism shifts from nutrient limitation cultivation to excess nutrient availability (and vice versa) conditions. Structured models, which are based on usage of some “intracellular physiological state markers” are needed to describe the “cell activity” thereby making model more robust in order to describe lag phase and dynamic culture cultivation conditions. Physiological state markers (such as RNA, Typical enzyme activity etc) provide intelligent correlation between the model simulation and experimental reality thereby enabling it to describe situations not possible by unstructured models.

#### **Basic features of Fermentation process –**

Fermentation process features cell cultivation in a suitable medium and ideal environmental conditions under aseptic conditions to facilitate higher growth which may lead to increased turnover of substrate to produce important metabolites. It can be classified as anaerobic cultivation of cells in which cells grow strictly in the absence of air particularly using metabolic intermediates as their final electron acceptors in the culture metabolism. Aerobic cultivation of cells, however, features vigorous growth of microorganisms in the presence of oxygen which acts as final electron acceptor. Higher growth of cells is achieved in aerobic cultivation than in anaerobic cultivation. In some cultivation the product of interest is accumulated with-in the cell (intracellular) and eventually the cell wall is ruptured to isolate and purify the product. Another variety of cultivation features extracellular

product formation in which substrate diffuses in to the cell, reacts with different enzymes to produce metabolites which is then excreted out of the cell in the fermentation broth. In this case cells are removed from the fermentation broth after the cultivation process and thereafter product isolation protocols e.g., extraction, distillation, precipitation etc are employed for harvesting the product from the fermentation broth.

### **Batch Microbial Cultivation and modeling –**

Batch cultivations are generally employed to grow cells for desired metabolite production as it is simple and involves least requirement of labor and equipments as opposed to other modes of cultivation (Fed-batch/ Continuous cultivations). However these cultivations work as closed system and thereby feature highly dynamic growth conditions and have less yield and productivity of desired product. This is particularly because of high non production time (Cleaning/Sterilization/Cooling etc) & due to significantly long Lag/Stationery phases in this mode of cultivation. Generally the higher activity featuring exponential growth (Balanced growth wherein all components of the cell grow by same proportion) of the culture is observed for only 25-40 % of total cultivation time of batch cultivation wherein the culture produces the metabolites of interest in growth associated fermentation processes. It is, therefore, desirable to study the culture growth and product formation characteristics (Kinetics) in detail and establish whether it is substrate or product inhibited system. If the kinetics turns out to be substrate inhibited (wherein, by increasing the initial substrate concentration in the bioreactor leads to significant decrease in growth) then it is desirable to design a fed-batch cultivation system such that higher initial substrate concentration in the bioreactor is replaced by gradual slow feeding of substrate such that at no point of time it reaches the inhibitory level. This will feature non limiting and non inhibitory nutrient availability cultivation conditions and result in increased product formation. If cultivation of growth in the presence of different product concentrations demonstrates slower growth at higher concentrations (product inhibition) then batch cultivation will not lead to higher rates of product formation as accumulated product will stay in the reactor and inhibit the growth. At significant higher product concentrations it may even stop the growth (and eventually product formation may cease) even under the conditions of high substrate (and associated nutrient) availability situations in the fermentation broth. To eliminate product inhibition growth conditions it is desirable to design either a plug flow or continuous reactor cultivations which features continuous feeding of nutrients and simultaneous withdrawal of fermentation broth along with the inhibitory product. Models are highly instrumental to design suitable reactors and their operation strategies to optimize any fermentation process.

**PROGRAM:****Function file:**

```
function fv=batch(t,y)

global um;
global ks;
global k1;
global k2;
global yxs;
global xi;
global si;
global pi;

fv(1,1)= ((um*y(2))/(y(2)+ks))*y(1);
fv(2,1)= -(((um*(y(2)))/(y(2)+ks))/(yxs))*y(1);
fv(3,1)= (k1+(k2*(um*y(2))/(y(2)+ks)))*y(1);
```

**Bmc file:**

```
function bmodel(t,y)
%Input data
disp('Enter the required input data according to the ranges.');
```

```
global um;
global ks;
global k1;
global k2;
global yxs;
global xi;
global si;
global pi;

um=input('um(0-1)=');
while(um<0 || um>1)
disp('Enter value within range');
um=input('um(0-1)');
end

ks=input('ks(0-50)=');
while(ks<0 || ks>50)
disp('Enter value within range');
ks=input('ks(0-50)=');
end

yxs=input('yxs(0-50)=');
while(yxs<0 || yxs>50)
disp('Enter value within range');
```

```

yxs=input('yxs (0-50)=');
end

k1=input('k1 (0-100)=');
while(k1<0 || k1>100)
disp('Enter value within range');
    k1=input('k1 (0-100)=');
end

k2=input('k2 (0-10)=');
while(k2<0 || k2>10)
disp('Enter value within range');
    k2=input('k2 (0-10)=');
end

xi=input('Enter the initial value of x, Biomass(g/l)=');
si=input('Enter the initial value of s, Substrate(g/l)=');
pi=input('Enter the initial value of p, Product(g/l)=');

ti=input('Define the initial time=');
tf=input('Define the final value time=');
ts=input('Define the step in time required=');

[tv,Yv]=ode45('batch',[ti:ts:tf],[xi;si;pi]);

Yv;

plot(tv,Yv(:,1),'-');
hold on
plot(tv,Yv(:,2),'-');
plot(tv,Yv(:,3),'-');
grid

title('Batch Microbial Cultivation : Model Equations');
xlabel('time (hrs)');
legend('X','S','P','Location','NorthEastOutside');

hold off
end

```

**OBSERVATION:**

**RESULT:**

**EXP NO: 4**

**DATE:**

**MODELING IN FED BATCH CULTURE IN MATLAB**

**AIM:**

To model microbial fed-batch growth kinetics in MATLAB

**THEORY**

**Fed-batch cultivation –**

The most simple category of fermentation is batch cultivation where in the substrate is taken in the beginning of cultivation and nothing is added or withdrawn during the fermentation.

However the yield and productivity is lower in these cultivations mainly because, either the substrate &/or product inhibition occurs and the product accumulation is never optimal. Fed-batch cultivation can provide the solution to substrate inhibition problem by slow feeding of nutrients to the bioreactor; however it can still not address the severe inhibition problem due to accumulating high product concentrations. The optimal design of fed-batch cultivation has to take in to account several factors in to consideration for example time to start the fresh nutrient feed (in the end or when the culture is exponentially growing) what should be the substrate concentration in the feed and its rate of addition and when to finish the nutrient feeding so that the highest concentration of product is produced and no unconverted substrate when the reactor is full. It is rather impossible to do trial and error experimentation with so many “open ended” variables (as described above) which may play key role in the overall performance of the fed-batch cultivation.

#### **Modelling of Fed-batch cultivation –**

A batch mathematical model is therefore developed using the kinetics of the fermentation which is extrapolated to fed-batch cultivation by incorporating the mass balance terms in the model equations. A large number of fed-batch simulations are then done off line by the developed model particularly to ensure that there is significant improvement in product formation and productivity by selection of high concentration of nutrients in the feed, during selected time periods, so that unnecessary dilution of the broth can be avoided and fresh feeding is done for maximum working volume of the reactor and also towards the end of fermentation the reactor should be having highest product concentration with no unconverted substrate.

#### **Different types of Fed-batch cultivation –**

Following scenario of nutrient feeding can contribute in the elimination of substrate inhibition to yield high productivity of the product.

#### **Add substrate when low –**

This is the simplest type of fed-batch cultivation where in the fresh feeding of the nutrient is done when substrate has become limiting towards the end of the batch cultivation. At this point of time if no feeding of fresh nutrient is done for some time, the culture dies out. A step input of substrate



(predesigned concentration and its rate) is identified by the mathematical model and is administered to the dying culture in the bioreactor which instantaneously raises the concentration of substrate and thereby gives an “installment” of life to the starving culture for few hours which results in product formation also for some more time than the batch cultivation. This cycle can be repeated number of times till the reactor is full of medium. In fact different combinations of substrate concentration, its rate and time of feeding can be chosen and used in the mathematical model to arrive at the best possible cultivation protocol for highly productive fermentation. The best offline simulated protocol can then be taken in to the lab and implemented to optimize the production.

**Constant feeding of substrate –**

Significant Improvement in product concentration and improvement in yield /productivity is possible if the nutrient feeding is done during the exponential phase of the cell growth when the maximum cell population is young and growing. This may be suitably selected by the study of batch kinetics. The mathematical model can then be used to simulate number of possibilities of start /stop time of nutrient feed, substrate concentration, its rate and so on. The simplest feeding profile could be constant feeding of suitably selected nutrient concentration and its pre identified rate such that it does not yield increased concentration of substrate than the initial substrate concentration at any time during the feeding in the bioreactor. Model can very easily facilitate the identification of above specific feeding strategy. The advantage of above strategy is that it is very simple it does not required computer coupled peristaltic pump to implement the feeding strategy. But the disadvantage is that it leads to build up of substrate which need to ferment by yet another batch cultivation so that in the end no unconverted substrate is left in the bioreactor.

**Linearly or exponentially increasing nutrient feeding strategy –**

In this fed-batch cultivation the nutrient feed is linearly or exponentially increased at predetermined time of cultivation. If the feeding rate coincides with the growth rate in the bioreactor by model simulations it may be possible to achieve non limiting non inhibitory concentration of substrate during the feeding period. However after the termination of feeding it may be necessary to do a secondary batch cultivation to consume the residual substrate in the bioreactor.

**Decreasing rate nutrient feeding strategy –**

The disadvantage of above feeding strategy can be overcoming by suitable selection of nutrient feeding strategy where in the feeding starts in exponential phase of fermentation and nutrient feeding

rate is so designed that feeding is high when the culture is young and there after the rate is gradually decreased as the culture gets older & is diluted by incoming feed nutrients. It is possible to arrive at a simulation where the feeding rate of nutrient gradually decreases & stops when the reactor is full. In this there will not be any requirement of secondary batch fermentation.

**Pseudo steady state of substrate or biomass –**

It is possible to design the nutrient feeding at a particular substrate concentration so that its concentration is neither high enough to inhibit the fermentation nor it is too low to limit the growth in the bioreactor. To arrive at the feeding profile, which might result the constant substrate concentration in the broth, the first derivative (say  $ds/dt$ ) is made zero and the model equations (because for S to be constant its first derivative has to be made zero) are rearranged to calculate the corresponding feeding rate of the substrate. The feeding of the nutrient thus calculated can then be implemented to achieve pseudo steady state of any variable e.g., S, X etc.

**Generalized feeding profile of nutrient feeding in fed-batch cultivation –**

In this type of fed-batch cultivation design the start/stop time of feeding is first identified and the nutrient feeding concentration rate / profile is so designed that it gives highest product concentration when the reactor is full at the end of the feeding. Non linear regression is used to find the coefficients of polynomial feeding profile, and the identified profile is then used with the model equations to simulate the maximum final product concentration. This may then be implemented experimentally to optimize the fermentation.

**PROGRAM:**

```
ic=[0.08; 25.0; 0.0; 2.2];
mumax=0.325;
Ks=1.12;
Yxs=0.65;
Ypx=0.25;
Sf=25.0;
mu = @(S) mumax*S/(Ks+S);
rg = @(X,S) mu(S)*X;
rp = @(X,S) Ypx*rg(X,S);
F = @(t) 0.05;
dXV = @(t,x) x(4)*rg(x(1),x(2));
dPV = @(t,x) x(4)*rp(x(1),x(2));
dSV = @(t,x) F(t)*Sf-x(4)*rg(x(1),x(2))/Yxs;
dV = @(t,x) F(t);
```

```

dX = @(t,x) (dXV(t,x) - x(1)*dV(t,x))/x(4);
dS = @(t,x) (dSV(t,x) - x(2)*dV(t,x))/x(4);
dP = @(t,x) (dPV(t,x) - x(3)*dV(t,x))/x(4);
f = @(t,x) [dX(t,x); dS(t,x); dP(t,x); dV(t,x)];
tspan = [0 30];
[t,x] = ode45(f,tspan,ic);
subplot(2,2,1);
plot(t,x(:,1));
xlabel('Time (hr)');
ylabel('X(g/L)');
title('Cell Concentration');
subplot(2,2,2);
plot(t,x(:,3));
xlabel('Time (hr)');
ylabel('P(g/L)');
title('Product Concentration');
subplot(2,2,3);
plot(t,x(:,2));
xlabel('Time (hr)');
ylabel('S(g/L)');
title('Cell Concentration');
subplot(2,2,4);
plot(t,x(:,4));
xlabel('Time (hr)');
ylabel('V(g/L)');
title('Volume');

```

**OBSERVATION:**

```

mumax    =    0.325
Ks        =    1.12
Yxs      =    0.65
Ypx      =    0.25
Sf        =    25.0

```

Initial Conditions:

```

X         =    0.08
S         =    25.0
P         =    0.0
V         =    2.2
Ti        =    0
Tf        =    30

```

**RESULT:**

**EXP NO:5**

**DATE:**

**MODELING IN CONTINUOUS CULTURE USING MATLAB**

**AIM:**

To model microbial continuous growth kinetics in MATLAB

**THEORY**

**Continuous Cultivation of microorganism –**

Continuous cultivation of microorganism are open systems which features addition of nutrients at a constant rate and simultaneous with drawl at the same rate. This mode of cultivation is particularly useful as it results in significant improvement in productivity of fermentation. Also it is rather easy to implement process control for these systems. However some disadvantages of this cultivation e.g, development of mutants and contamination free cultivation for longer time limits its common usage. However it is a best tool to study the physiology of cultivation as there is a perfect steady state cultivation condition at a particular dilution rate (= sp. growth rate) in the bioreactor.

**Transients in Chemostats –**

The overall response of any continuous cultivation can be simulated by the mathematical model however it is rather interesting to see the culture behavior in transients in cultivation (Shift up / Shift down in dilution rates) It has been observed that Monod model is unable to perfectly simulate the transients in Continuous cultivations because the model assumes dependence of growth on the instantaneous value of substrate concentration. In shift up of dilution rates (i.e., increasing the feeding rate of nutrient) the metabolism switches from “famine” condition to “feast” condition, meaning suddenly the substrate concentration see a significant change against the nutrient limiting / dying culture and there is no proportionate increase in the cell growth as proposed by Monod’s model. It is therefore necessary to incorporate the “physiological state marker” in the model which

can not only quantitatively describe the metabolic reactions of the cells but adequately graduate changes in nutrient limiting and nutrient rich situations in transient conditions of continuous cultivations. The transients are particularly important in microbial cultivations as it may lead to significant increase in the product concentrations which are not available elsewhere. This is particularly important because the culture experiences a major shift in nutrient availability and thereby it leads to quick change over of the culture metabolism.

### Wash out condition –

In any cultivation it is always necessary to devise strategies which might result in high productivity. Productivity in continuous cultivation is dependent on not only the concentration of biomass /product but also on its dilution rate (Productivity =  $DP$  or  $DX$ ). It is therefore necessary to increase both  $D$  and  $X$  to increase the productivity of fermentation. However in actual practice, it is observed that at lower dilution rate, unconverted substrate is low & biomass concentration is high (Productivity = High Biomass x Low  $D$ ) and on the contrary at high dilution rates, unconverted substrate is high & biomass concentration is low. (Productivity = Low Biomass x High  $D$ ). Therefore in either of the two cases the multiplication of  $DX$  results in lower productivity. Also if dilution rate of the bioreactor is further enhanced then it may lead to “wash out” of the biomass from the reactor. The substrate concentration in the reactor will then be equal to the inlet concentration of feed substrate. For optimization of the productivity, suitable Dilution rate ( $D_{\text{maxout put}}$ ) is identified which when used during cultivation conditions gives best value of steady state biomass accumulation in the bio reactor there by increasing the productivity. It is also possible to improve the process productivity by using cell retention / recycle system which allow build up of biomass in the bioreactor and it becomes possible to operate the reactor at higher dilution rates ( $D = \text{Feed rate/Volume}$ ) with-out wash out.

### PROGRAM:

```
ic=[0.01; 10; 0.0];
mumax=0.3;
Ks=0.1;
Yxs=0.8;
k1=0.1;
k2=0.3;
Sf=10;
mu = @(S) mumax*S/(Ks+S);
rg = @(S,X) mu(S)*X;
rs=@(S,X) -rg(S,X)/Yxs;
rp = @(S,X) (((k1+k2)*mu(S))*X);
D = @(S) mumax*(1-(Ks/(Ks+S))^0.5);
```

```
dX = @(t,x) ((-x(1)*D(x(2)))+rg(x(2),x(1)));
dS = @(t,x) (-D(x(2))*(Sf-x(2)) + rs(x(2),x(1)));
dP = @(t,x) ((-D(x(2))*x(3)) + rp(x(2),x(1)));
f = @(t,x) [dX(t,x); dS(t,x); dP(t,x)];
tspan = [0 30];
[t,x] = ode45(f,tspan,ic);
subplot(2,2,1);
plot(t,x(:,1));
xlabel('Time (hr)');
ylabel('X(g/L)');
title('Cell Concentration');
subplot(2,2,2);
plot(t,x(:,3));
xlabel('Time (hr)');
ylabel('P(g/L)');
title('Product Concentration');
subplot(2,2,3);
plot(t,x(:,2));
xlabel('Time (hr)');
ylabel('S(g/L)');
title('Substrate Concentration');
xlabel('Time (hr)');
ylabel('S(g/L)');
```

**OBSERVATION:**

mumax	=	0.3
Ks	=	0.1
Yxs	=	0.8
k1	=	0.1
k2	=	0.3
Sf	=	10
Initial Conditions:		
X	=	0.01
S	=	10
P	=	0.0
Ti	=	0
Tf	=	30

**RESULT:**

**EXP NO: 6**

**DATE:**

## MODELING IN PRODUCT FORMATION USING MATLAB

### AIM:

To model product formation kinetics in MATLAB

### Theory:

#### **Basic concepts & need of Acetone – Butanol - Ethanol production from renewable resources**

Fluctuations and continuous upward trend in the price as well as uncertainty of a reliable steady supply of hydrocarbon feed stocks have a profound effect on petrochemical markets. Alternative manufacturing processes are being sought based preferably on renewable raw materials. Fermentation-based fuel processes & industrial solvent production processes are being re-examined for their potential in supplying these materials “competitively priced” & in an “environmentally” safe manner. While anaerobic product oriented fermentation processes have been known since the beginning of this century their industrial exploitation reached its peak between the World wars. New hopes are placed in the bioconversion processes and based on the rapidly changing hydrocarbon feedstock situation, recent breakthroughs in the development of superior microbial catalysts and on significant improvements in fermentation technologies coupled together with advanced process control and product recovery techniques. Last but not the least; it is the renewable resources which they are capable of utilizing which makes bioconversion processes so attractive. Not only can the renewable resource materials be utilized but a number of dilute waste streams originating from other manufacturing sectors constitute perfect raw materials for production of desirable compounds based on fermentation processes.

During the recent era of pressing energy shortage the process of acetone-butanol biosynthesis the fermentative production of higher alcohols (butanol, iso-propanol) and ketones (acetone) by bacterial strains has received relatively little attention as yet. Indeed, bacterial anaerobic product yielding processes in general are not so well understood and received only very scattered contemporary scientific attention, particularly when it comes to their more sophisticated industrial scale-up and utilization. This is partly due to the difficulties associated with the investigation of strictly anaerobic microbial strains.

This bacterium is characterized by easy growth on a variety of substrate, synthesizing three major liquid end products (A-B-E) through two intermediate acids (acetic and butyric) giving off a gaseous

mixture of CO<sub>2</sub> and H<sub>2</sub> (Rogers, 1986). The culture features a complex metabolism (at pH 4.5, Temperature 37°C by rod shaped bacteria) and an intriguing physiology reflected in a stage-wise fermentation and a spore forming life cycle. A normal batch fermentation is characterized by acid production during its first acidogenic phase which is followed by a solventogenic phase when most of the acids are reabsorbed and solvents accumulate to the point of process termination (2 %) due to their toxicity. The young growing culture in the acid fermentation phase does not possess the enzymatic apparatus for reducing the acids. The most important productive second phase of the culture features a low growth rate solvent production and acid uptake. The long time it takes for the development of the solvent production phase is partially responsible for the low overall productivity of the batch fermentation. Appropriate conditions for solvent production are sought in order to improve the solvent productivity. All of these features and the sensitivity of the strain to environmental factors make it a challenging target for in-depth study.

However, apart from the theoretical challenges of the process, there exist very strong practical and economic stimuli for increased scientific attention to the anaerobic product-oriented microbial processes. Some of these stimuli are listed below

**PROGRAM:**

```
ic=[100; 0.1; 0.1; 0.01; 0.01; 0.004; 0.1]; %S,Ba,Aa,B,A,E,X
um=0.678;
Ks=30;
Ki=17.07;
Y=0.06042;
m=0.002;
k1=0.75;
k2=3.53;
k3=0.3395;
k4=2.26;
k5=0.01;
k6=0.951;
k7=0.0861;
k8=0.1;
k9=0.01372;
Kba=0.272;
Kaa=0.793;
Kd=0;

mu = @(S,B) um*(S/(S+Ks))*(Ki/(Ki+B))-Kd*B;
rs=@(S,B) ((1/Y)*um*(S/(S+Ks))*(Ki/(Ki+B))-Kd*B)+m;
dx = @(t,x) (um*(x(1)/(x(1)+Ks))*(Ki/(Ki+x(4)))-Kd*x(4))*x(7);
```



```

dS = @(t,x) -(rs(x(1),x(4)))*x(7);
dC=      @(t,x) (k1*rs(x(1),x(4))-
(k2*(x(2)/(x(2)+Kba))* (Ki/(Ki+x(4)))))*x(7);
dD=      @(t,x) (k3*rs(x(1),x(4))-
(k4*(x(3)/(x(2)+Kaa))* (Ki/(Ki+x(4)))))*x(7);
dB=      @(t,x) (k5*rs(x(1),x(4))-
(k6*(x(2)/(x(2)+Kba))* (Ki/(Ki+x(4)))))*x(7);
dA=      @(t,x) (k7*rs(x(1),x(4))-
(k8*(x(3)/(x(3)+Kaa))* (Ki/(Ki+x(4)))))*x(7);
dE= @(t,x) k9*rs(x(1),x(4))*x(7);
f = @(t,x) [dS(t,x); dC(t,x); dD(t,x); dB(t,x); dA(t,x); dE(t,x);
dX(t,x)];
tspan = [0 5];
[t,x] = ode45(f,tspan,ic);
subplot(3,3,1);
plot(t,x(:,1));
xlabel('Time (hr)');
ylabel('S(g/L)');
title('Substrate Concentration');
subplot(3,3,2);
plot(t,x(:,2));
xlabel('Time (hr)');
ylabel('Ba(g/L)');
title('Ba');
subplot(3,3,3);
plot(t,x(:,3));
xlabel('Time (hr)');
ylabel('Aa(g/L)');
title('Aa');
subplot(3,3,4);
plot(t,x(:,4));
xlabel('Time (hr)');
ylabel('B(g/L)');
title('B');
subplot(3,3,5);
plot(t,x(:,5));
xlabel('Time (hr)');
ylabel('A(g/L)');
title('A');
subplot(3,3,6);
plot(t,x(:,6));
xlabel('Time (hr)');
ylabel('E(g/L)');
title('E');
subplot(3,3,7);
plot(t,x(:,7));
xlabel('Time (hr)');
ylabel('X(g/L)');
title('Cell Concentration');

```

**OBSERVATION:**

um = 0.678  
Ks = 30  
Ki = 17.07  
Y = 0.06042  
M = 0.002  
k1 = 0.75  
k2 = 3.53  
k3 = 0.3395  
k4 = 2.26  
k5 = 0.01  
k6 = 0.951  
k7 = 0.0861  
k8 = 0.1  
k9 = 0.01372  
Kba = 0.272  
Kaa = 0.793  
Kd = 0

Initial Conditions:

S = 100  
Ba = 0.1  
Aa = 0.1  
B = 0.01  
A = 0.01  
E = 0.004  
Ti = 0  
Tf = 50

**RESULT:**

**EXP NO: 7**

**DATE:**

**MODELLING OF BATCH CULTURE BY BERKELEY-MADONNA**

**AIM:**

To model microbial batch growth kinetics in BERKELEY-MADONNA

**Theory:**

Berkeley Madonna is the fastest, most convenient general purpose differential equation solver available today. It is relatively inexpensive and runs on both Windows and Mac OS. Developed on the Berkeley campus under the sponsorship of NSF and NIH, it is currently used by academic and commercial institutions for constructing mathematical models for research and teaching. A version of

Berkeley Madonna, called JMadonna, is in development. It will have the user interface written in Java, while retaining the simulation engine in C for speed. This will allow us to extend Berkeley Madonna in many ways, including a Linux version.

**The Runge–Kutta model:**

One member of the family of Runge–Kutta methods is often referred to as "RK4", "classical Runge–Kutta method" or simply as "*the* Runge–Kutta method".

Let an initial value problem be specified as follows.

$$\dot{y} = f(t, y), \quad y(t_0) = y_0.$$

Here,  $y$  is an unknown function (scalar or vector) of time  $t$  which we would like to approximate; we are told that  $\dot{y}$ , the rate at which  $y$  changes, is a function of  $t$  and of  $y$  itself. At the initial time  $t_0$  the corresponding  $y$ -value is  $y_0$ . The function  $f$  and the data  $t_0, y_0$  are given. RK4 model was used in Berkely Madonna software to analyze the various growth parameters in batch, fed batch and continuous cultures.

**Sailent features of Berkley Madonna software:**

- Used to solve ordinary differential equation
- Easy to use
- Very fast execution
- Sensitivity analysis- plots the partial derivative of any variable with respect to any parameter
- Fast Fourier transform - plot results in frequency domain.

**PROGRAM:**

```
METHOD RK4

STARTTIME = 0
STOPTIME=70
DT = 0.02
d/dt (X)=RX
d/dt (S)=RS
d/dt (P)=RP
RX=U*X
```

```
U=UM*S / (KS+S)
RS=-RX/Y
RP= (K1+K2*U) *X
init X=1
init S=100
init P=0
K1=0.005
K2=0.002
Y=0.8
KS=0.1
UM=0.03
```

**OBSERVATION:**

```
mumax      =    0.03
Ks          =    0.1
k1          =    0.005
k2          =    0.002
Initial Conditions:
X           =    1
S           =   100
P           =    0.0
Ti          =    0
Tf          =   70
```

**RESULT:**

**EXP NO: 8**

**DATE:**

**CONTINUOUS MODEL IN BERKELEY-MADONNA**

**AIM:**

To model microbial continuous growth kinetics in BERKELEY-MADONNA

**Theory:**

Berkeley Madonna is the fastest, most convenient general purpose differential equation solver available today. It is relatively inexpensive and runs on both Windows and Mac OS. Developed on the Berkeley campus under the sponsorship of NSF and NIH, it is currently used by academic and commercial institutions for constructing mathematical models for research and teaching. A version of Berkeley Madonna, called JMadonna, is in development. It will have the user interface written in Java, while retaining the simulation engine in C for speed. This will allow us to extend Berkeley Madonna in many ways, including a Linux version.

**The Runge–Kutta model:**

One member of the family of Runge–Kutta methods is often referred to as "RK4", "classical Runge–Kutta method" or simply as "*the* Runge–Kutta method".

Let an initial value problem be specified as follows.

$$\dot{y} = f(t, y), \quad y(t_0) = y_0.$$

Here,  $y$  is an unknown function (scalar or vector) of time  $t$  which we would like to approximate; we are told that  $\dot{y}$ , the rate at which  $y$  changes, is a function of  $t$  and of  $y$  itself. At the initial time  $t_0$  the corresponding  $y$ -value is  $y_0$ . The function  $f$  and the data  $t_0, y_0$  are given. RK4 model was used in Berkely Madonna software to analyze the various growth parameters in batch, fed batch and continuous cultures.

**Sailent features of Berkley Madonna software:**

- Used to solve ordinary differential equation
- Easy to use
- Very fast execution
- Sensitivity analysis- plots the partial derivative of any variable with respect to any parameter
- Fast Fourier transform - plot results in frequency domain.

**PROGRAM:**

METHOD RK4

STARTTIME = 0

STOPTIME=30

DT = 0.02

$d/dt (X) = -D \cdot X + RX$

$d/dt (S) = -D \cdot (Sf - S) + RS$

$d/dt (P) = -D \cdot P + RP$

$d/dt (Xa) = D \cdot X + ta \cdot C \cdot D \cdot X + U \cdot X - (1 + ta) \cdot D \cdot X$

$RX = U \cdot X$

$U = UM \cdot S / (KS + S)$

$RS = -RX / Y$

$RP = (K1 + K2 \cdot U) \cdot X$

init X=0.01

initXa=0.01

init S=10

init P=0

K1=0.1

K2=0.3

KS=0.1

Y=0.8

UM=0.3

Sf=10

ta=0.05

**OBSERVATION:**

mumax = 0.3

Ks = 0.1

Yxs = 0.8

k1 = 0.1

k2 = 0.3

Sf = 10

Initial Conditions:

X = 0.01

S = 10

P = 0.0

Ti = 0

Tf = 30

**RESULT:**

**EXP NO: 9**

**DATE:**

**PRODUCT KINETICS BY BERKELEY-MADONNA**

**AIM:**

To study the model for product formation kinetics using Berkeley Madonna.

**Theory:**

Berkeley Madonna is the fastest, most convenient general purpose differential equation solver available today. It is relatively inexpensive and runs on both Windows and Mac OS. Developed on the Berkeley campus under the sponsorship of NSF and NIH, it is currently used by academic and commercial institutions for constructing mathematical models for research and teaching. A version of Berkeley Madonna, called JMadonna, is in development. It will have the user interface written in Java, while retaining the simulation engine in C for speed. This will allow us to extend Berkeley Madonna in many ways, including a Linux version.

**The Runge–Kutta model:**

One member of the family of Runge–Kutta methods is often referred to as "RK4", "classical Runge–Kutta method" or simply as "*the* Runge–Kutta method".

Let an initial value problem be specified as follows.

$$\dot{y} = f(t, y), \quad y(t_0) = y_0.$$

Here,  $y$  is an unknown function (scalar or vector) of time  $t$  which we would like to approximate; we are told that  $\dot{y}$ , the rate at which  $y$  changes, is a function of  $t$  and of  $y$  itself. At the initial time  $t_0$  the corresponding  $y$ -value is  $y_0$ . The function  $f$  and the data  $t_0, y_0$  are given. RK4 model was used in Berkeley Madonna software to analyze the various growth parameters in batch, fed batch and continuous cultures.

**Sailent features of Berkeley Madonna software:**

- Used to solve ordinary differential equation



- Easy to use
- Very fast execution
- Sensitivity analysis- plots the partial derivative of any variable with respect to any parameter
- Fast Fourier transform - plot results in frequency domain.

**PROGRAM:**

METHOD RK4

STARTTIME = 0

STOPTIME=5

DT = 0.02

$u = u_m * (S / (s + K_s)) * (K_i / (K_i + B)) - K_d * B$

$d/dt(x) = (u_m * (S / (s + K_s)) * (K_i / (K_i + B)) - K_d * B) * x$

$rs = (1/Y) * u_m * ((S / (s + K_s)) * (K_i / (K_i + B)) - K_d * B) + m$

$d/dt(s) = -rs * x$

$d/dt(Ba) = (k_1 * rs - (k_2 * (Ba / (Ba + K_{ba})) * (K_i / (K_i + B)))) * x$

$d/dt(Aa) = (k_3 * rs - (k_4 * (Aa / (Ba + K_{aa})) * (K_i / (K_i + B)))) * x$

$d/dt(B) = (k_5 * rs - (k_6 * (Ba / (Ba + K_{ba})) * (K_i / (K_i + B)))) * x$

$d/dt(A) = (k_7 * rs - (k_8 * (Aa / (Aa + K_{aa})) * (K_i / (K_i + B)))) * x$

$d/dt(E) = (k_9 * rs) * x$

um=0.678

Ks=30

Ki=17.07

Y=0.06042

m=0.002

k1=0.75

k2=3.53

k3=0.3395

k4=2.26

k5=0.01

k6=0.951

k7=0.0861

k8=0.1

k9=0.01372

Kba=0.272

Kaa=0.793

Kd=0

init s=100

init Ba=0.1

initAa=0.1

init B=0.01

init A=0.01

init E=0.004

**OBSERVATION:**

um = 0.678  
Ks = 30  
Ki = 17.07  
Y = 0.06042  
M = 0.002  
k1 = 0.75  
k2 = 3.53  
k3 = 0.3395  
k4 = 2.26  
k5 = 0.01  
k6 = 0.951  
k7 = 0.0861  
k8 = 0.1  
k9 = 0.01372  
Kba = 0.272  
Kaa = 0.793  
Kd = 0

Initial Conditions:

S = 100  
Ba = 0.1  
Aa = 0.1  
B = 0.01  
A = 0.01  
E = 0.004  
Ti = 0  
Tf = 50

**RESULT:**

EXP NO: 10

DATE:

**SIMULATION BY SIMULINK IN BATCH CULTURE**

**AIM:**

To model microbial batch growth kinetics using simulink

**PROGRAM:**

- Open SIMULINK in MATLAB
- Setup the model using the blocks with the model equations as reference
- Connect the output of each variable to the scope block to get a graph output

$$V \frac{dX}{dt} = r_X V$$

$$V \frac{dS}{dt} = r_S V$$

$$V \frac{dP}{dt} = r_P V$$

$$r_X = \mu X$$

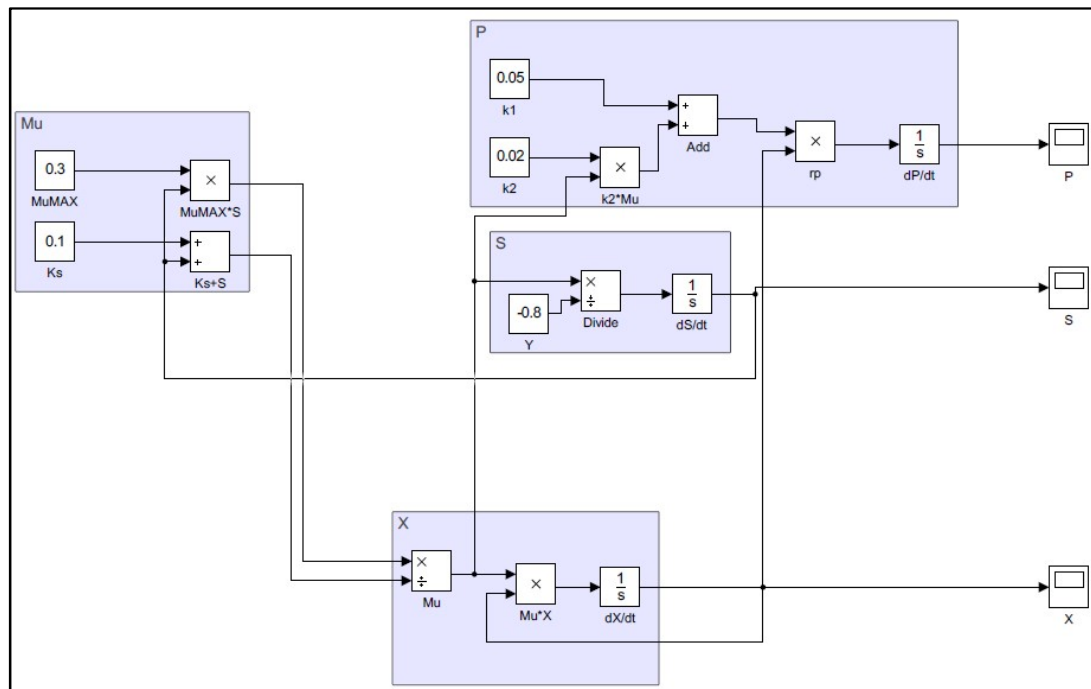
$$\mu = \frac{\mu_m S}{K_S + S}$$

$$r_S = -\frac{\mu}{Y_{X/S}}$$

$$r_P = (k_1 + k_2 \mu) X$$

init X =100, init S = 9, init P = 0, K1 =0.05, K2 =0.02, Y=0.8, KS=0.1, UM=0.3

**MODEL :**



**OBSERVATION:**

**RESULT:**

EXP NO: 11

DATE:

**SIMULATION BY SIMULINK IN CONTINUOUS CULTURE**

**AIM:**

To model microbial continuous growth kinetics using simulink

**PROGRAM:**

- Open SIMULINK in MATLAB
- Setup the model using the blocks with the model equations as reference
- Connect the output of each variable to the scope block to get a graph output

FOR CELLS  $\frac{dX}{dt} = -DX + r_X$

$r_X = \mu X$

FOR SUBSTRATES  $\frac{dS}{dt} = -D(S_F - S) + r_S$

$\mu = \frac{\mu_m S}{K_s + S}$

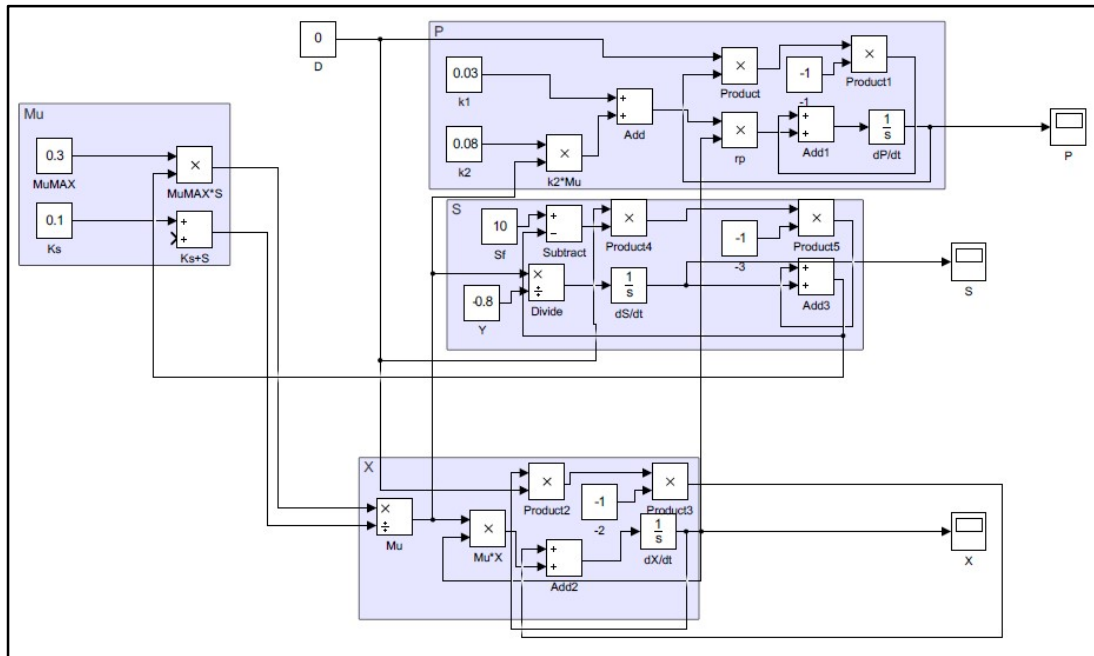
FOR PRODUCTS  $\frac{dP}{dt} = -DP + r_P$

$r_S = -\frac{\mu}{Y_{X/S}}$

$r_P = (k_1 + k_2 \mu) X$

Time period = 18 h, init X =0.01, init S = 10, init P = 0, init V=1, K1 =0.03,K2 = 0.08, Y = 0.8, KS = 0.1, UM = 0.3, SF = 10, D=0

**MODEL :**



**OBSERVATION:**

**RESULT:**

EXP NO: 12

DATE:

**SIMULATION IN FED BATCH MODEL USING SIMULINK**

**AIM:**

To model microbial Fed-Batch growth kinetics by simulink

**PROGRAM:**

- Open SIMULINK in MATLAB
- Setup the model using the blocks with the model equations as reference
- Connect the output of each variable to the scope block to get a graph output

$$\text{Total Balance } \frac{dV}{dt} = F$$

$$\text{For Cells } \frac{d(V, X)}{dt} = r_x V$$

$$\text{For Substrate } \frac{d(V, S)}{dt} = FS_F + r_s V$$

$$\text{For Product } \frac{d(V, P)}{dt} = r_p V$$

$$r_x = \mu X$$

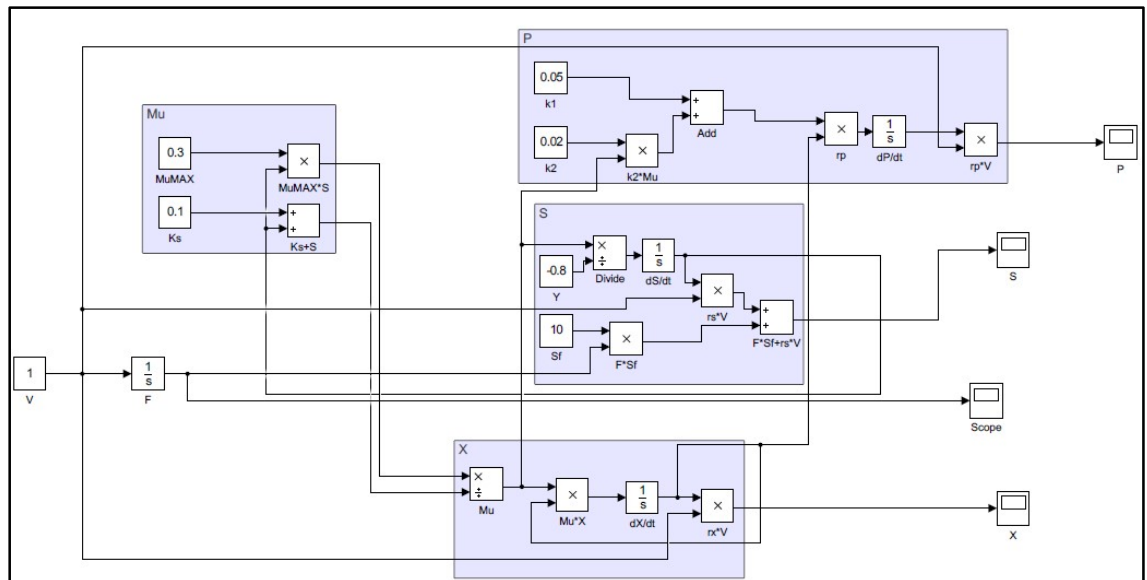
$$\mu = \frac{\mu_{max} S}{K_s + S}$$

$$r_s = -\frac{\mu}{Y_{X/S}}$$

$$r_p = (k_1 + k_2 \mu) X$$

Time period = 18 h, init X =0.01, init S = 10, init P = 0, init V=1, K1 =0.03, K2 = 0.08, Y = 0.8, KS = 0.1, UM = 0.3, SF = 10, D=F/V

**MODEL :**



**OBSERVATION:**

**RESULT:**



**EXP NO: 13**

**DATE:**

**SOLVING MATERIAL BALANCE USING SUPERPRO DESIGN**

**AIM:**

To solve material balance using super pro design.

**THEORY:**

Super pro designer facilitates modeling, evaluation and optimization of integrated process in a wide range of industries(pharmaceutical,biotech,speciality chemical,food,consumer goods, mineral processing,microelectronics,water purification,waste water treatment).The combination of manufacturing and environmental operation models in the same package enables the user to concurrently design and evaluate manufacturing and end of pipe treatment processes and practice waste minimization via pollution prevention as well as pollution control.

Superpro design is a valuable tool for engineers and scientists in process development, process engineering and manufacturing.It is also a valuable tool for professionals dealing with environmental issues.Process modeling capabilities, including:

- Generation of material and energy balances
- Environmental impact calculations
- Resource tracking
- Process scheduling
- Equipment sizing and costing
- Capital and operating cost estimation

In addition to producing various types of charts, SuperPro generates a variety of reports that summarize the equipment utilization, material usage, economic results, etc. These reports provide additional details about the process for engineers, scientists, managers, and operators. For instance, the Materials and

Streams report gives an overall summary of the process, breaks down the total amount of each material required per year, batch, or kg of main product, and gives the compositions and physical properties of each individual stream. Other material balance reports available from SuperPro provide information that is specific to emissions reporting and liquid and solid wastes.

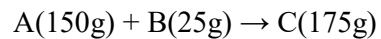
**PROCEDURE:**

1. Start a new process file and select batch operation.
2. Click Task and select pure components and register heptane and add new components as A, B, C.
3. Type A with its component name as sucrose, type B with component name water and type c and click ok.
4. Set mass balance for each component and enter the molecular weight as 150 for A, 25 for B, 175 for c by selecting physical constraint and process time as 30 minutes and click ok.
5. Reaction parameters:  
Temperature-50°C, Heat Agent-Steam, Set up time-15mins, reaction time-60 mins, conversion-100%.
6. Select unit process  $\Rightarrow$  Batch vessel procedure  $\Rightarrow$  Reactor and click anywhere on the screen.
7. Select unit process  $\Rightarrow$  Filtration  $\Rightarrow$  plate and frame filter and click it.
8. In reactor select charge and rename it as charge 1 as charge heptane, charge2 as reactant A, charge 3 as reactant B and select Transfer to PFF-101.
9. Click filtration, select wash cake, click transfer out. Right click and select  $\Rightarrow$  Edit tag name  $\Rightarrow$  S-101  $\Rightarrow$  Heptane ok.
10. Set parameters for heptanes loading: volume: 1200L, set time: 15mins, process time: 30 mins vent emission: Heptane.
11. Click molar  $\Rightarrow$  set extent: 95  $\Rightarrow$  transfer out: ~~#0 S-105~~  $\Rightarrow$  set percent:100  $\Rightarrow$  set up time:15mins  $\Rightarrow$  set by master slave reaction set up.
12. Filtration condition: set time: 15mins, process time: 4 hours, cake LOD-35%.

13. Transfer out: Mass-817kg, Volume-100L, user time-30min-PFF 2 and check mass balance for the process.
14. Right click style  $\implies$  edit style  $\implies$  info tag location  $\implies$  vertical near destination and click ok.
15. Save the file in pdf format.
16. The summary and outputs like Gantt chart, Equipment Occupancy Chart, Resource Demand (Purified Water), Labor Demand, Resource Inventory (WFI), Material Balance Report, Financial Reports are retrieved.

**Result:**

Using superpro design, mass balance with chemical reaction in batch process was solved



The following outputs were obtained:

- 1) Material and Stream Report (SR)
- 2) Economic Evaluation Report (EER)
- 3) Cash flow analysis (CFR)
- 4) Itemized Cost Report (ICR)
- 5) Throughput Analysis Report (THR)
- 6) Environmental Impact Report (EIR)
- 7) Emission Report (EMS)
- 8) Equipment Report (ER)
- 9) CIP Skid (CSR)
- 10) Input Data Report (IDR)
- 11) Excel Custom Report
- 12) Gantt Chart

