

**Aspects of Biochemical Engineering**  
**Prof. Debabrata Das**  
**Department of Biotechnology**  
**Indian Institute of Technology, Kharagpur**

**Lecture - 23**  
**Kinetics of Enzyme Catalyzed Reactions Using Free Enzymes – III**

Welcome back to my course aspects of biochemical engineering, and last couple of lectures I try to concentrate on enzymes that I told you what do you mean by enzymes and what is the classification of enzymes, then I try to tell that what we mean by inhibition of the enzymes, and also that you know when we talk about the enzymatic reaction kinetics. The major thing that comes with that is the Michaelis Menten equation with largely use and how the Michaelis Menten proposed their equation; later on vixen hold helen they justify this Michaelis Menten equation with the help of reaction kinetics, then question comes how the enzymatic reaction constant like  $v_{max}$  and  $k_m$  can be estimated with the help of 3 different plots. One is locking k hypothesis another is proximity effect another is orientation effect.

The inhibition is the very important part because through inhibition we can apply this enzyme for enzymatic reaction kinetics for the estimation of the different complex molecules, also it can be used for protection our healths to kill this certain infection. So, this is the different type of inhibition, we talked about the reversible inhibition, we talked about the irreversibility inhibition and finally, we discussed that that substrate inhibition how substrate inhibition can be taken into account. Now today actually you can remember that when we discuss about the reactor analysis, we have come across 3 different type of processes one is batch process, this CHTA, and then plug flow reactor.

Now, those we have solve for the chemical process. Now when we apply to the enzymatic reaction system, how we can determined that batch time, and how you would determine the space time for CSTR using enzymes, and how you determine to and the space time for the plug flow reactor and finally, I want to discuss one problem. And with the help of reactor analysis how it is possible to find out the reactor. Suppose we want to produce a certain amount of product and for getting the this the product and using the same enzymes, whether batch reacted will required less volume or CSTR will required

less volume or plug flow reactor that this question will be answered in one numerical problems.

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**Enzymatic reaction in batch process**

- ✓ Batch is an unsteady state operation
- ✓ Material balance for substrate can be given as:

Input + Generation = Output + Consumption + Accumulation

$$0 = (-r_s)V + \frac{d(SV)}{dt}$$

As working volume (V) is constant,

$$-\frac{d(S)}{dt} = v = \frac{V_{max}S}{K_m + S} \dots(1)$$

As  $v = -r_s = \frac{V_{max}S}{K_m + S}$

The slide includes a diagram of a batch reactor with a stirrer. The substrate concentration is labeled as  $S_0$ . Handwritten notes include  $q_s \rightarrow -\frac{ds}{dt} \frac{mass}{vol}$  and a circled equation  $v = -r_s = \frac{V_{max}S}{K_m + S}$ . The slide footer identifies the speaker as DEBABRATA DAS, DEPARTMENT OF BIOTECHNOLOGY, IIT KHARAGPUR.

So, first let me start with this how we can analyze this enzymatic reaction or the batch processes. So, we when we talk about the batch process batch process we considered as the unsteady state process why?

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The slide shows handwritten diagrams. On the left, a grid represents substrate concentration (S) over time (t), with axes labeled  $S_1, S_2, S_3, S_4$  and  $t_1, t_2, t_3, t_4$ . A circled equation  $-\frac{ds}{dt} = r_s = k(S)$  is written above the grid. On the right, a diagram of a reactor shows substrate (S) and enzyme (E) entering, and substrate (S) leaving. Below it, a graph shows substrate concentration (S) versus time (t).

Because that this is the reactor, and in this reactor this is the substrate you take. So, you pull put your substrate here, and put your enzyme here let the reaction take place and we

can draw the sample from here and we can monitor what is the substrate concentration at different times that we can monitor. And when you plot that concentration of substrate versus time if we plot this plot, then what will happen with respect to time that substrate concentration will be decreases.

Now, if you make a slope at different points, then what will get? You will get minus  $dS$  by  $dt$  what is  $dS$  minus  $dS$  by  $dt$  is the rate of reaction, how you can really express this?  $R_s$ ;  $r_s$  is the rate of reaction and this is. So, you know this is equal to if we consider this is the first order reaction this is the  $k$  into  $s$ . So, that you know that had different time this is  $t_1$  this is  $t_2$ , this is  $t_3$ , this is  $t_4$ . So, at different time we have different substrate concentration. So, this is  $s_1$ , this is  $s_2$ , this is  $s_3$ . So, as the substrate concentration is changes your rate of reaction changes and since the rate of reaction changes we consider it as the unsteady state conditions.

So, this is exactly what we want to point out that batch system is considered as the unsteady state reaction. Now if you do the material analysis when you go back to the reactor analysis, we use one particular equation what is that equation? Rate of input plus rate of generation equal to rate of output, plus rate of disappearance, plus rate of accumulation. So, this is how this equation looks like this. Now in case of batch process there is no input. So, input is equal to 0 output also equal to 0, now there is no generation because substrate is consumed. So, what will happen 2 things simultaneously check place one is consumption and the accumulation.

So, this will be like this what is the consumption rate of consumption of substrate we can write minus  $r_s$  into  $v$ . Why minus  $r_s$  into  $v$ , I explained before also minus  $r_s$  is equal to what? Equal minus  $dS$  by  $dt$  am I right. So, what is  $dS$ ?  $Ds$  is the concentration what is the concentration? This is mass per unit volume. So, the well, but when you do the balance; balance across the whole reactor this and your reaction take place in the liquid phase only. So, we shall have to multiply this  $r_s$  with  $v$  to consider all the reaction that take place in the reaction mixture. So, this will be like this and what will be the rate of accumulation of substrate  $s$  into  $v$   $d, s$  into  $v$  by  $dt$  now when you differentiate this,  $v$  is constant the volume of the reactor is constant.

So, it will come out. So, it will be  $dS$  by  $dt$ . So, I can write minus  $dS$  by  $dt$  equal to  $v$  equal to that minus  $r_s$  and then this is as far Michaelis Menten equation, this will be

equal to  $v_{max} \frac{s}{K_m + s}$ . Now here we have shown  $v$  equal to  $\frac{v_{max} s}{K_m + s}$ . So, this is very simple that we can determine the correlation between we can make a balanced equation across the batch reactor. Now when we do this analysis of this equation that I can show you that is like this, now what we have we have  $-\frac{ds}{dt}$  this will be equal to Michaelis Menten equation velocity of (Refer Time: 08:05)  $v_{max} \frac{s}{K_m + s}$  am I right.

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$$-\frac{ds}{dt} = \frac{v_{max}s}{K_m + s}$$

$$-ds(K_m + s) = v_{max} \cdot dt$$

$$-K_m ds - s ds = v_{max} dt$$

$$\int_{s_0}^s \frac{1}{s} ds - \frac{ds^2}{2} = \int_{0}^t v_{max} dt$$

$$\ln\left(\frac{s_0}{s}\right) - \frac{s^2 - s_0^2}{2} = v_{max} t$$

$$\ln\left(\frac{s_0}{s}\right) = \frac{v_{max}}{K_m} t$$

Now, this what I can do I can take  $-\frac{ds}{dt} = \frac{v_{max}s}{K_m + s}$ , I can write and this is I can write  $v_{max}$  equal to  $v_{max} \frac{s}{K_m + s}$  into  $dt$ . Now  $s$  I can bring it this side, then rub it here and I can bring it this side  $s$  and this is  $dt$ . Now if you solve it what you will get? You can get I can write  $1$  by  $v_{max}$ , I can  $v_{max}$  I can take this side,  $v_{max}$  I can take common, this will be equal to  $K_m$  into  $-\ln\left(\frac{s}{s_0}\right) = \frac{v_{max}}{K_m} t$ . So, you can write minus because minus will come here and this is will be  $-\ln\left(\frac{s}{s_0}\right)$  this will be  $-\ln\left(\frac{s}{s_0}\right)$  am I right.

So, these this will cancel and. So, this will be equal to  $dt$ ; now this how we can write? This is  $v_{max} - K_m$  now what is this  $\ln$ , this we can write  $\ln\left(\frac{s_0}{s}\right) - \frac{s^2 - s_0^2}{2} = v_{max} t$ . And now we can do the integration, now what is the integration I can do? This is a  $\int_{s_0}^s \frac{1}{s} ds$  and here also  $\int_{s_0}^s ds$  and here this is equal to  $dt$ , this also we can  $0$  to  $t$ . Now if you do that then we will come across the equation what  $1$  by  $v_{max}$  equal to  $K_m \ln\left(\frac{s_0}{s}\right)$  because this was minus.

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$$\frac{1}{v_{max}} \left( \frac{k_m S}{S_0 - S} + S_0 \right) = t_{batch}$$

$$\frac{1}{v_{max}} \left( \frac{k_m (1 - x_s)}{0.5} + \frac{x_s S_0}{0.5} \right) = \frac{t_{batch}}{S_0 - S}$$

$$x_s = \frac{S_0}{S_0 - S}$$

$$1 - \frac{S}{S_0} = (1 - x_s)$$

So, I can always make it you know reverse. So, it will be plus, and here it is minus this is S minus s 0.

Now, if you plus then it will be S 0 minus S this will be equal to like this, this will be equal to t then this is called batch time. So, if you know the value of k m and v max and you know that what is the percentage of substrate consumption is there, then you can easily find it out. Now one thing I want to point out sometime, I we can express in terms of x a x s. X s is what? The fraction of S that is converted how we can express this S 0 minus S by S 0 am I right this is fraction of x that is converted.

Now, I want to write this through here what I can write this is 1 minus S by S 0 equal to x s. So, I can write S by S 0 equal to 1 minus x s this we can write. So, this equation I can modified as v max k m l n, 1 minus x s and then here also we can write in the form of x s because then S 0 minus s equal to x s into S 0 it equal to t batch. Now why we are we are interested for that? Suppose we want to convert 50 percent of substrate just we put it to a 0.5 x s equal to 0.5 here, and you know initial substrate concentration we can put the value of k m we can easily find out the value of t batch .

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### Enzymatic reaction in batch process

Integrating Eq. (1)

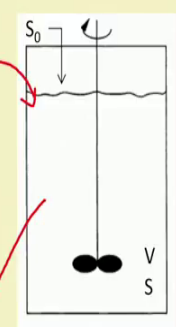
$$\int_{S_0}^S \frac{K_m + S}{S} dS = \int_0^{t_b} -V_{max} dt$$


$$\int_{S_0}^S \frac{K_m}{S} dS + \int_{S_0}^S dS = -V_{max} \int_0^{t_b} dt$$

$$V_{max} \ln \frac{S}{S_0} + (S - S_0) = -V_{max} t_b$$


$$V_{max} t_b = K_m \ln \frac{S_0}{S} + (S_0 - S) \text{ i. e. } t_b = \frac{1}{V_{max}} \left[ K_m \ln \frac{S_0}{S} + (S_0 - S) \right]$$

The total batch reaction time ( $t_{Tb}$ )

$$t_{Tb} = t_b + t_{dn} \quad (\text{where } t_{dn} \text{ is the Down time for preparation, harvesting, cleaning etc.})$$




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Now, similar thing has been written here this is how finally, we derived this equation, this is there is a  $t_b$  batch;  $t_b$  batch is coming at we will be like this and this will be little bit problem this will be like this. So, some mistake is there you can correct it, and the total batch time will be equal to batch time total time of the batch process is the batch time plus downtime what do you mean by downtime? Time required for taking out the liquid and time required to clean the vessel, and time required to refill the vessel that is we considered as the downtime and what is the; what do you mean by that you know downtime means there is no reaction.

So, sometime downtime also we call it the idle time, idle what is idle time? Idle time means no reaction take place, that is why we call it idle time.

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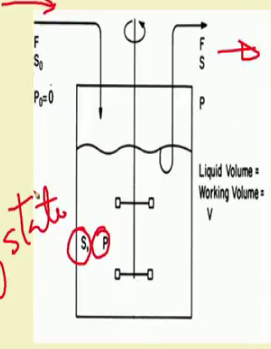
### Enzymatic reaction in continuous stirred tank reactor (CSTR)

- ✓ CSTR may be operated at a **steady state condition**
- ✓ The rate of substrate degradation depends upon:
  - Volumetric flow rate (**F**) and
  - Dilution rate (**D**)

$$D = \frac{F}{V} \text{ (time}^{-1}\text{)}$$

Hydraulic retention time  $\text{HRT} = \frac{1}{D}$

- ✓ Material balance for substrate can be written as  
Input + Generation = Output + Consumption + Accumulation

$$FS_0 + 0 = FS + (-r_s)V$$


The diagram shows a CSTR with an inlet stream on the left labeled with flow rate  $F$  and substrate concentration  $S_0$ . The inlet pressure is  $P_0 = 0$ . Inside the reactor, there is a stirrer and a liquid level. The outlet stream on the right is labeled with flow rate  $F$  and substrate concentration  $S$ . The outlet pressure is  $P$ . The liquid volume is labeled as  $V$ . Handwritten red text 'Batch' and 'Steady state' with arrows points to the inlet and outlet respectively. A circled 'S' is also present near the outlet.

Liquid Volume = Working Volume =  $V$

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So, this is how we can find out the batch process the time required for the batch process, now if you come to the continuous process the situation is little bit simpler, and batch that that this process is very easy to operate you can see this is the reactor, and here I told you whenever you operate any kind of continuous stirred tank reactor, first you have to operate it in a batch mode. First you operate in a batch mode and then let the reaction take place when you get the maximum rate of reaction, then you continuously feed the substrate and take out the product from the other end. And then when you operate for infinite period of time you will find the concentration of substrate and concentration of product remain constant and that we consider as the steady state.

Stay what is. So, what do you mean by steady state? With the steady state means when the concentration and different parts of the reactor remains unaltered that is called steady state.

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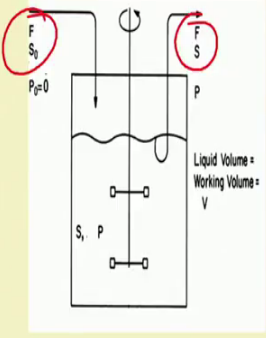
### Enzymatic reaction in continuous stirred tank reactor (CSTR)

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$$D = \frac{F}{V} \text{ (time}^{-1}\text{)}$$

Hydraulic retention time  $HRT = \frac{1}{D}$


Material balance for substrate can be written as  
~~Input + Generation = Output + Consumption + Accumulation~~  
 $FS_0 + 0 = FS + (-r_s)V$



Liquid Volume = Working Volume = V



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Now here that the CSTR may be operated under steady state condition, rate of substrate degradation depends on flow rate and the dilution rate. Now what is dilution rate? Dilution rate is nothing, but F by V what is the F is the volumetric flow rate, volumetric flow rate means volume per unit time am I right now this is equal to volume.

So, V is the unit is volume. So, V V will cancel. So, it will time. So, the unit will be D what is the unit of D? Time inverse HRT is the hydraulic retention time equal to 1 by D high what is hydraulic retention time? Hydraulic detentions the how long you allow the liquid to reside in the reactor. Now how you can we can do the material analysis the same formula we can have rate of input plus rate of generation, equal to rate of output the consumption accumulation now since we had doing the substrate balance. So, in case of substrate knows product substrate generation is there. So, we can write rate of input Fequal to S 0, what is the output F into S; F into S is the output you can see, this is the input that we have and what is the consumption of substrate minus r s into V.



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### Enzymatic reaction in CSTR

$$F(S_0 - S) = \left( \frac{V_{max}S}{K_m + S} \right) V$$

As  $v = -r_s = \frac{V_{max}S}{K_m + S}$

$$D(S_0 - S) = \frac{V_{max}S}{K_m + S} \quad (\text{since } D = \frac{F}{V})$$

The above equation can be used to calculate dilution rate required to reach particular substrate conversion

Substrate conversion =  $\frac{S_0 - S}{S_0}$

$\tau = \frac{1}{D} = \frac{V}{F} = \frac{V_{max}S}{K_m(S_0 - S)}$

$\tau_{CSTR} = \frac{S_0 - S}{\frac{V_{max}S}{K_m}}$

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Now, if you would write this equation we can write this equation in this form, that F; this equation we have this form and this equation we have if you look at this equation with the F 0 into equal to F s plus minus r s; r s velocity of reaction what is velocity of reaction? This you can expressed as V max s divided by K m plus S. Now this is exactly what we have written here and. So, this is final expression will be like this that f V the V I can take it this side. So, this will be d the dilution rate into S 0 minus S equal to V max S this is we can. So, this is equal to this, and this seem the dilution rate that you know that is like this.

So, 1 by d is the hydraulic retention time. So, from that I can easily find out that what is the space time required in this reactor, how we can find out let me show you. This suppose we can write this, this is equal to D equal to I can write. What I can write D equal to V max S divided by k m plus S am I right. Now this is divided by 1 by S 0 minus s and what is this? This is equal to I can write this is the dilution rate equal to F by D and 1 by D is equal to what? Where the HRT and this is the actually HRT is nothing, but space time of the CSTR; that means, how we express tau CSTR. So, how you can write the expression this is inverts. So, how you can write the tau CSTR? Tau CSTR will be equal to S 0 minus S divided by v max s k m plus S.

So, we can easily find out this tau CSTR now let me talk about this Plug flow reactor.

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### Enzymatic reaction in plug flow reactor (PFR)

- ✓ PFR may also be operated continuously under steady state condition
- ✓ There is **no axial mixing, only radial mixing**
- ✓ **Material balance** for substrate in small section ( $\Delta Z$ )

Input + Generation = Output + Consumption + Accumulation

$$FS \Big|_z = FS \Big|_{z+\Delta z} + (-r_S)A\Delta z$$

Rearranging the above equation

$$\frac{F(S \Big|_z - S \Big|_{z+\Delta z})}{A\Delta z} = -\frac{v_{max}S}{K_m + S}$$

$$\frac{u(S \Big|_z - S \Big|_{z+\Delta z})}{\Delta z} = -\frac{v_{max}S}{K_m + S}$$

$As$   
 $v = -r_S = \frac{v_{max}S}{K_m + S}$

Superficial velocity  
 through the column,  $u = \frac{F}{A}$

$A$  - Cross-sectional area of the  
 reaction  
 $F$  - Volumetric flow rate  
 $v = -r_S = \frac{v_{max}S}{K_m + S}$

$dV = A\Delta z$

Now plug flow reactor I told you it is also can be operated under steady state conditions that, but you know plug flow reactor plug flow I to what I told, you that plug flow is not there something similar to the piston flow. What do you mean by piston flow? Piston flow is the ideal flow suppose there is the piston here and when a piston goes the we assume the velocity across this cross section is the uniform, but actual case when liquid pass through any kind of table tube, then we have gradient of velocity. We have like this we have gradient or will do as the liquid close to the wall surface then the velocity will be reduced.

Why it is reduced? Due to the friction between the liquid and the wall surfaces there is the friction and due to the friction the velocity of the liquid will be reduces to a great extent. So, and the, but that is in case of piston flow, the is considered as the ideal flow because the we assume there is no velocity gradient across the cross section of this. Now in a true sense when you have laminar flow we have velocity gradient across the cross section of the tube, but when you a an angular flow tends to the turbulent flow, then velocity gradient will be minimized.

Now, how you can do this analysis of the reactor? Here we have this is suppose this is the reactor that we have.

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### Enzymatic reaction in plug flow reactor (PFR)

- ✓ PFR may also be operated continuously under steady state condition
- ✓ There is no axial mixing, only radial mixing
- ✓ **Material balance** for substrate in small section ( $\Delta Z$ )

Input + Generation = Output + Consumption + Accumulation

$$FS|_z = FS|_{z+\Delta z} + (-r_S)A\Delta z$$

Rearranging the above equation

$$\frac{F(S|_{z+\Delta z} - S|_z)}{A\Delta z} = -\frac{v_{max}S}{K_m + S}$$

$$\frac{u(S|_{z+\Delta z} - S|_z)}{\Delta z} = -\frac{v_{max}S}{K_m + S}$$

$As$   
 $v = -r_S = \frac{v_{max}S}{K_m + S}$

Superficial velocity through the column,  $u = \frac{F}{A}$

$A$ - Cross-sectional area of the reaction  
 $F$ - Volumetric flow rate  
 $v = -r_S = \frac{v_{max}S}{K_m + S}$

$dV = A\Delta z$

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This is the input one end, I told you in this there is no back mixing no axial mixing is there or, but there will be radial mixing. Suppose radial mixing means suppose this is a tube and here you can have radial mixing, circular there will be mixing, but there is no mixing in the axis; that is actually there taking place. Now for analysis this reactor what do you do? We take a differential segment this is the differential segment, where we this is the F that is the input and what is the F is the flow rate in, F is the flow rate out.

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### Enzymatic reaction in plug flow reactor (PFR)

- ✓ PFR may also be operated continuously under steady state condition
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- ✓ **Material balance** for substrate in small section ( $\Delta Z$ )

Input + Generation = Output + Consumption + Accumulation

$$FS|_z = FS|_{z+\Delta z} + (-r_S)A\Delta z$$

Rearranging the above equation

$$\frac{F(S|_{z+\Delta z} - S|_z)}{A\Delta z} = -\frac{v_{max}S}{K_m + S}$$

$$\frac{u(S|_{z+\Delta z} - S|_z)}{\Delta z} = -\frac{v_{max}S}{K_m + S}$$

$As$   
 $v = -r_S = \frac{v_{max}S}{K_m + S}$

Superficial velocity through the column,  $u = \frac{F}{A}$

$A$ - Cross-sectional area of the reaction  
 $F$ - Volumetric flow rate  
 $v = -r_S = \frac{v_{max}S}{K_m + S}$

$dV = A\Delta z$

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But substrate here substrate concentration is the  $S_z$ , here  $S_z \Delta z$ ,  $\Delta z$  is the width of the particular differential unit. So, I can write  $F$  into  $S_z$  that is the rate of input of substrate  $F$  into  $S_z$  plus  $\Delta z$  is the output and minus  $r_s$  into  $A$ ,  $A$  is the area cross sectional area if you multiplied by this into  $\Delta z$  you will get the volume of this volume if we assume to be  $\Delta V$ ,  $\Delta V$  equal to nothing, but equal to  $\Delta z$  into  $A$ . So, I can write it  $\Delta V$  is equal to  $\Delta z$  into  $A$ ,  $A$  is the cross sectional area.

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**Enzymatic reaction in plug flow reactor (PFR)**

- ✓ PFR may also be operated continuously under steady state condition
- ✓ There is **no axial mixing, only radial mixing**
- ✓ **Material balance** for substrate in small section ( $\Delta Z$ )

Input + Generation = Output + Consumption + Accumulation

$$F S \Big|_z = F S \Big|_{z+\Delta z} + (-r_s) A \Delta z$$

Rearranging the above equation

$$\frac{F(S \Big|_{z+\Delta z} - S \Big|_z)}{A \Delta z} = -\frac{v_{max} S}{K_m + S}$$

$$\frac{u(S \Big|_{z+\Delta z} - S \Big|_z)}{\Delta z} = -\frac{v_{max} S}{K_m + S}$$

As  $v = -r_s = \frac{v_{max} S}{K_m + S}$

Superficial velocity through the column,  $u = \frac{F}{A}$

$dV = A \Delta z$

A - Cross-sectional area of the reaction  
 F - Volumetric flow rate  
 $v = -r_s = \frac{v_{max} S}{K_m + S}$   
 $dV = A \Delta z$

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So, this is a nothing, but the volume of the reactor and if you solve it, it will come in this particular form and then we again we if we do the integration that of this.

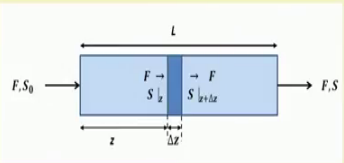


volume is the length cubed. So, this will cancel will be length, length by time is equal to the velocity. So, this is exactly that we have shown here, and then if we if we do this, this will be equal to u into limit this a this can be integrated and this equation will comes like this and finally, we come across this is the equation that we have, that is the u into d S by d z equal to v max S by K m plus s and this is equal to 1 by u where that d z equal to this one.

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**Enzymatic reaction in PFR**

$$\frac{V}{F} = \frac{L}{u} = \frac{1}{v_{max}} \left\{ K_m \ln \left( \frac{S_0}{S} \right) + (S_0 - S) \right\}$$

$$\tau_{PFR} = \frac{V}{F} = \frac{L}{u} = \frac{1}{v_{max}} \left\{ K_m \ln \left( \frac{S_0}{S} \right) + (S_0 - S) \right\}$$


The space time of PFR is same as time required for batch reactor for a particular reaction

$$t_{batch} = \tau_{PFR}$$

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And finally, that we have this equation  $L$  by  $u$  equal to  $1$  by  $v_{max}$ , and by this now I want to point out  $L$ ;  $L$  means length am I right and what is  $u$  is the velocity length per unit time. So, what will happen that if we this length will cancel and this is equal to nothing, but tau plug flow reactor. And this is  $1$  by  $v_{max} k_m S_0$  and if you look at this equation it is same as compared to the batch process. Batch process we have the similar expression with that. So, that is why we have been written the space time and the space time of plug flow reactor same as required the batch process for the particular reaction.

(Refer Slide Time: 25:33)

**Problem:** Glucose is to be converted to fructose by using glucose isomerase enzyme, initial glucose concentration in the reaction mixture is 200 g/L, the degree of conversion 60% w/w.

Calculate the volume needed to produce 10 kg of fructose per day by glucose isomerase in a

- Batch reactor ✓
- CSTR ✓
- Plug flow reactor ✓

Data

- Michaelis-Menten reaction kinetics with  $v_{max} = 1.5 \times 10^{-2} \text{ kg s}^{-1} \text{ m}^{-3}$  biocatalyst and  $K_m = 5 \text{ kg m}^{-3}$
- $Y_{P/S} = 1 \text{ kg kg}^{-1}$
- Down-time for batch reactor 4 h
- The activity of the biocatalyst can be assume to be constant in time

(P)

G → F

Now, I want to show you the solution of a particular problem to make this things very clear, because the final objective of the reactor analysis just to find out the volume of the reactor. Now this is a very interesting problem the glucose is converted to fructose by using glucose isomerase enzyme, initial glucose concentration in the reaction mixture is 200 grams per liter, degree of conversion is 60 percent, calculate the volume needed for 10 kg fructose production. Now the enzyme we use glucose isomerase what is the happening the glucose is converted to fructose? And fructose is 10 times greater than glucose.

So, this is used largely in the confectionery industry to convert glucose into fructose now. So, with this particular reaction, we want to find out which reactor will be good in the batch reactor CSTR and plug flow reactor. And these are the different values that is  $v_{max}$  and  $k_m$  value and other value this given in the problem.



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**Problem:** Glucose is to be converted to fructose by using glucose isomerase enzyme, initial glucose concentration in the reaction mixture is 200 g/L. the degree of conversion 60% w/w. Calculate the volume needed to produce 10 kg of fructose per day by glucose isomerase in a


- Batch reactor
- CSTR
- Plug flow reactor

Data

- Michaelis-Menten reaction kinetics with  $v_{max} = 1.5 \times 10^{-2} \text{ kg s}^{-1} \text{ m}^{-3}$  biocatalyst and  $K_m = 5 \text{ kg m}^{-3}$
- $Y_{P/S} = 1 \text{ kg kg}^{-1}$
- Down-time for batch reactor 4 h
- The activity of the biocatalyst can be assume to be constant in time

**Solution:**

**Given stoichiometry:** Glucose (S)  $\xrightarrow{\text{E}}$  Fructose (P)



Now the basic stoichiometry of this equation is like this the one mole of glucose produce one mole of fructose this is the stoichiometry we have.

(Refer Slide Time: 26:40)

**Given data,** initial substrate concentration,  $S_0 = 200 \text{ g/L} = 200 \text{ kg/m}^3$   
 degree of conversion,  $X_S = 0.60$   
 $v_{max} = 1.5 \times 10^{-2} \text{ kg s}^{-1} \text{ m}^{-3}$   
 $K_m = 5 \text{ kg m}^{-3}$   
 $Y_{P/S} = 1 \text{ kg kg}^{-1}$   
 downtime,  $t_d = 4 \text{ h}$

**i. Batch reactor**

It is known that,  $t_{batch} = -\int_{S_0}^S \frac{dS}{(-r_S)}$   
 as it follows M-M kinetics  $(-r_S) = \frac{v_{max}S}{K_m + S}$

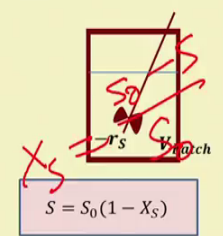

Integration yields

$$t_{batch} = \frac{1}{v_{max}} [-K_m \ln(1 - X_S) + X_S S_0]$$

Putting all the known values

$$t_{batch} = \frac{1}{1.5 \times 10^{-2}} [-5 \ln(1 - 0.60) + 0.60 \times 200] = 8305.43 \text{ s}$$

$\approx 2.307 \text{ h}$

Now then the batch reactor what we have already derived this equation am I right that in the batch we have this. So, now, v max value is given here, k m value is given here X I show have shown you X s what is x? Xs is the fraction of substrate that is converted this is the S by S 0 am I right.



So, I have shown you this. So, if you put this value directly, you will get this is the volume of the reactor is coming 2.3 hours, and then we can find out that total time.

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$t_{total} = t_{batch} + t_{down\ time}$   
 $t_{total} = 2.307 + 4 = 6.307\ h$   
 Now, no. of batch per day =  $\frac{24}{6.307} = 3.80$   
 Base: 10 kg of fructose (P) per day  
 Product to be produced per batch =  $\frac{10}{3.80} = 2.63\ kg$   
 As,  $Y_{P/S} = 1\ kg\ kg^{-1}$ , substrate required per batch = 2.63 kg  
 For  $X_S = 0.60$ , actual substrate required per batch =  $\frac{2.63}{0.60} = 4.38\ kg$   
**Volume of reactor required** =  $\frac{\text{actual substrate required}}{\text{initial substrate concentration}} = \frac{4.38\ kg}{200\ \frac{kg}{m^3}} = 0.022\ m^3$   
 $= 22\ L$   
 ii. CSTR  
 $\tau_{CSTR} = \frac{S_0 - S}{(-r_S)} = \frac{(S_0 - S)(K_m + S)}{(v_{max}S)} = \frac{S_0 X_S \{K_m + S_0(1 - X_S)\}}{v_{max} S_0 (1 - X_S)}$   
 $\tau_{CSTR} = \frac{0.60 \times \{5 + 200(1 - 0.60)\}}{1.5 \times 10^{-2} \times (1 - 0.60)}$   
 $\tau_{CSTR} = 8500\ s = 2.36\ h$   
 200 g/L → 200 kg/m³

What is the total time? The batch time plus idle time idle time means 4 hours the total is that. Now one when we want to calculate the volume of the batch first we shall have to find out how many batch you have to operate per day. The this is 3.8 batches. So, you have how much product you have to produce 10 kg of fructose, the per batch how much product is to be produced is divide by 3 point 8.

So, you will 2.63 kg of product and for this product how much substrate is required? Glucose it required 2.6 because one gram of glucose produced one gram of fructose. So, 60 percent conversion of substrate is there. So, you can easily find out how much glucose is required for the batch process. Now if you know then how much glucose is required for the batch process and this is the initial concentration of substrate. The concentration of substrate was 20 gram per liter and this can be expressed as 20 kg per cubic meter. So, this is the exactly what we actually done and this is coming at 0.022 cubic meter.

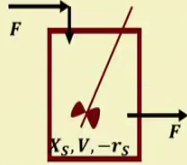
So, what is the volume is coming in the batch process is 22 liters. Now when you come to the CSTR tau CSTR that we have already derived this equation,  $S_0$  minus  $s$  minus  $r$  s then put this equation, in this form put this way we find this time required for the CSTR goes is 2.36 that hours.

(Refer Slide Time: 29:00)

$t_{total} = t_{batch} + t_{down\ time}$   
 $t_{total} = 2.307 + 4 = 6.307\ h$   
 Now, no of batch per day =  $\frac{24}{6.307} = 3.80$   
 Base: 10 kg of fructose (P) per day  
 Product to be produced per batch =  $\frac{10}{3.80} = 2.63\ kg$   
 As,  $Y_{P/S} = 1\ kg\ kg^{-1}$ , substrate required per batch = 2.63 kg  
 For  $X_S = 0.60$ , actual substrate required per batch =  $\frac{2.63}{0.60} = 4.38\ kg$   
**Volume of reactor required** =  $\frac{\text{actual substrate required}}{\text{initial substrate concentration}} = \frac{4.38\ kg}{200\ \frac{kg}{m^3}} = 0.022\ m^3$   
 $= 22\ L$

ii. CSTR  
 $\tau_{CSTR} = \frac{S_0 - S}{(-r_S)} = \frac{(S_0 - S)(K_m + S)}{(v_{max}S)} = \frac{S_0 X_S \{K_m + S_0(1 - X_S)\}}{v_{max} S_0 (1 - X_S)}$   
 $\tau_{CSTR} = \frac{0.60 \times \{5 + 200(1 - 0.60)\}}{1.5 \times 10^{-2} \times (1 - 0.60)}$   
 $\tau_{CSTR} = 8500\ s = 2.36\ h$

$S = S_0(1 - X_S)$



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Then we find.

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Base: 10 kg of fructose (P) per day  
 For  $Y_{P/S} = 1$ , substrate required per day =  $10\ \frac{kg}{d}$   
 As  $X_S = 0.60$ , actual substrate required per day =  $\frac{10\ kg}{0.60\ day} = 16.67\ \frac{kg}{d}$   
 Actual substrate required per hour =  $\frac{16.67\ kg}{24\ h} = 0.70\ \frac{kg}{h}$   
**Volumetric flow rate (F)** =  $\frac{\text{actual substrate required}}{\text{initial substrate concentration}} = \frac{0.70\ \frac{kg}{h}}{200\ \frac{kg}{m^3}} = 3.5 \times 10^{-3}\ \frac{m^3}{h}$

Now, we know  $\tau_{CSTR} = \frac{V_{CSTR}}{F}$   
 $V_{CSTR} = F \times \tau_{CSTR} = 3.5 \times 10^{-3} \times 2.36\ m^3 = 8.26 \times 10^{-3}\ m^3 = 8.26\ L$

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Out that how much product you have to produce 10 kg per day am I right? 10 kg product per day we are for the 10 kg product how much substrate is required? 60 percent conversion of substrate though you divide by 0.6. So, it is coming 16.767 kg per day.

Though per day; that means, how much substrate is consumed per hour? You divide by 24 hours because one day is 24 hour. So, it is coming 0.7 kg per hour. So, and. So, how much actual substrate is required this, and what is the initial substrate concentration? 200

kg per cubic meter and what is the volume we get? This is about 3.6 into this is the below that flow rate we get, and we if we this flow rate will be multiplied by CSTR tau CSTR will get the volume, and volume we are getting 8.26. So, from this we can conclude that when you operate the continuous process, the volume of the reactor is drastically reduced, that you can easily find out from these calculations.

(Refer Slide Time: 30:17)

**iii. Plug flow reactor (PFR)**

It is known that,  $\tau_{PFR} = - \int_{S_0}^S \frac{dS}{(-r_S)}$

as it follows M-M kinetics  $(-r_S) = \frac{v_{max}S}{K_m + S}$

Integration yields  $\tau_{PFR} = \frac{1}{v_{max}} [-K_m \ln(1 - X_S) + X_S S_0]$

Putting all the known values  $\tau_{PFR} = \frac{1}{1.5 \times 10^{-2}} [-5 \ln(1 - 0.60) + 0.60 \times 200] = 8305.43 \text{ s}$

$= 2.307 \text{ h}$

Base: 10 kg of fructose (P) per day

For  $Y_{P/S} = 1$ , substrate required per day = 10  $\frac{\text{kg}}{\text{d}}$

As  $X_S = 0.60$ , actual substrate required per day =  $\frac{10 \text{ kg}}{0.60 \text{ d}} = 16.67 \frac{\text{kg}}{\text{d}}$

Actual substrate required per hour =  $\frac{16.67 \text{ kg}}{24 \text{ h}} = 0.70 \frac{\text{kg}}{\text{h}}$

$S = S_0(1 - X_S)$

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Now, similarly we can do the calculation for the plug flow reactor, we have this equation and this is similar to your batch process. So, same time you will get, but only thing is that the conversion of this with respect to this that similar to as CSTR. So, we find out how much substrate is required, same amount of substrate required per hour this way this we can easily find out and then flow rate the same flow rate what do you observe for CSTR as the same flow rate will get.

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Volumetric flow rate ( $F$ ) =  $\frac{\text{actual substrate required } \frac{\text{kg}}{\text{h}}}{\text{initial substrate concentration } \frac{\text{kg}}{\text{m}^3}} = \frac{0.70 \text{ m}^3}{200 \text{ h}}$   
 $= 3.5 \times 10^{-3} \frac{\text{m}^3}{\text{h}}$

Now, we know  $\tau_{PFR} = \frac{V_{PFR}}{F}$   
 $V_{PFR} = F \times \tau_{PFR} = 3.5 \times 10^{-3} \times 2.307 \text{ m}^3 = 8.07 \times 10^{-3} \text{ m}^3 = 8.07 \text{ L}$

	Batch reactor	CSTR	PFR
Volume (L)	22	8.26	8.07

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Now the this flow rate if you multiplied with taus plug flow reactor will get the volume.

So, in salt if you find out that if you summarize all the all the things, then what will get? We will get the volume in case of batch process is coming 22 hours in CSTR, 8.26 and plug flow reactor 8.07; that means, the our design should be plug flow reactor because if we recommend what reactor is suitable for this process, we should go for plug flow reactor. So, what I conclude in this lecture that, this is vital in the sense that how this reactor analysis can be apply in the enzymatic reaction system, and we here also we try to analyze both batch reactor CSTR and the plug flow reactor and we have taken and we try to find out the mathematical equation, with respect to t batch with respect to tau CSTR with respect to tau.

Plug flow reactor and once you we have that then we can easily find out for a for producing a certain amount of product how much time is required for the batch process, how much time is required for the continuous CSTR, and plug flow reactor that we can easily find out. And once we know the time then we shall have to in case of continuous process we shall have to find out the flow rate then we can find out the volume of the reactor. And when you compare all this and whatever which reactor which process having the lower the smaller size, that will be our design of the reactor this is how we can design the reactor.

Thank you very much.