Chemical Reaction Engineering-I
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Lecture - 13
Ideal Plug Flow Reactor Design

Welcome to the third lecture of module 4. In this module we are discussing reactor design for single reaction.

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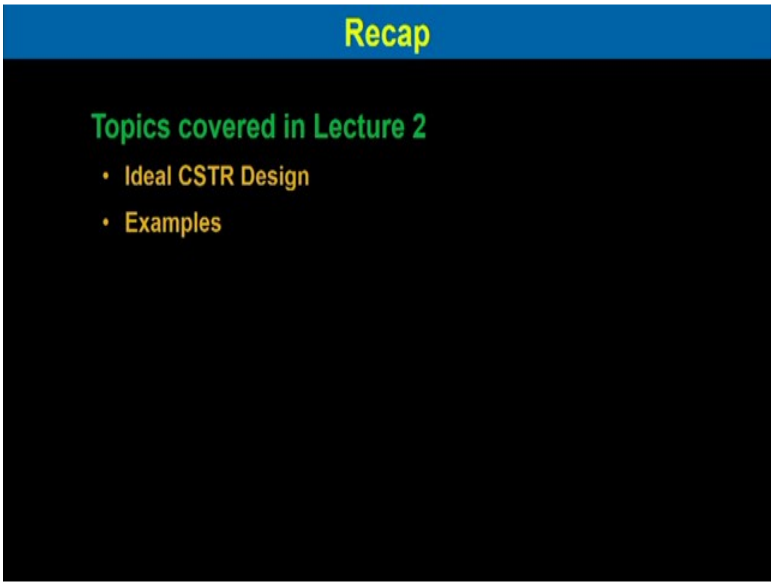

Recap

Topics covered in Lecture 2

- Ideal CSTR Design
- Examples

Before going to this lecture let us have brief recap on our previous lecture, in the previous lecture we have merely covered ideal CSTR design and then we have tried to see different examples to calculate the volume or kinetics of the reactions, how to find out the kinetics using the CSTR.

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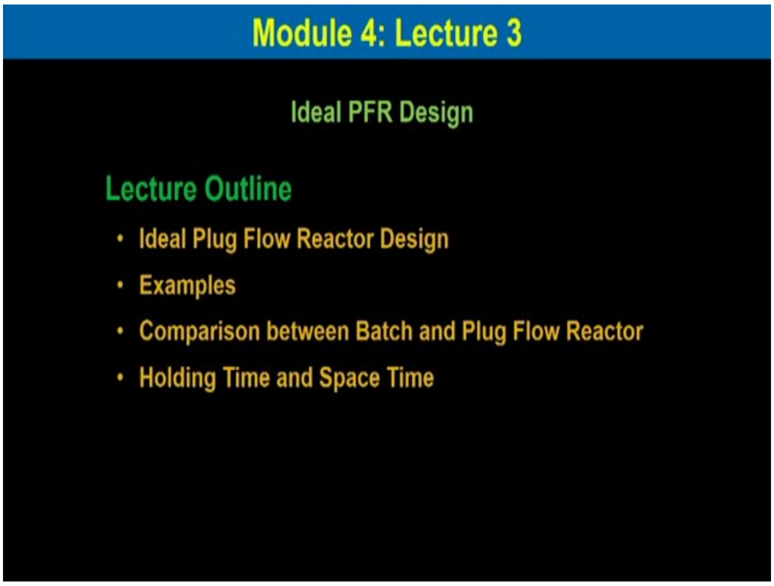

Module 4: Lecture 3

Ideal PFR Design

Lecture Outline

- Ideal Plug Flow Reactor Design
- Examples
- Comparison between Batch and Plug Flow Reactor
- Holding Time and Space Time

In this lecture we will consider ideal Plug Flow Reactor design. The lecture outline would be ideal Plug Flow Reactor design, then we will see examples how to calculate the volume of the reactor for a particular operation and then we will compare between Batch and Plug Flow Reactor, and then finally we will see the holding time and space time for flow reactor.

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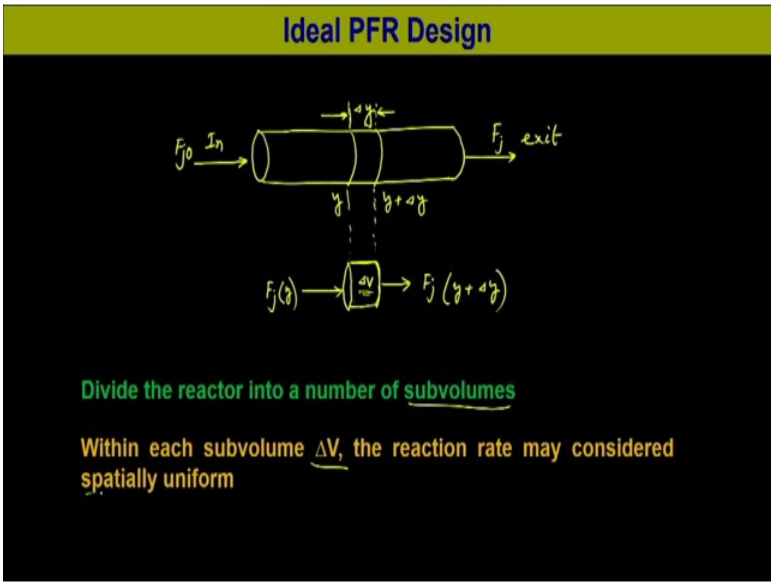

Ideal PFR Design

Divide the reactor into a number of subvolumes

Within each subvolume ΔV, the reaction rate may considered spatially uniform

So ideal Plug flow Reactor design, so before going to this ideal plug flow design let us look back the earlier two reactors which we have covered, one batch reactor, another is mixed flow reactor. So batch reactor we have seen that it is used for small scale industries and it has certain advantage and disadvantages, but mostly it is used for small scale production. But in this case we have used stirring into the system although it is a close system, we use stirring and so the content inside the reactor each homogeneous at any time.

In case of the mixed flow reactor that is the flow reactor where we have feed in and then product out. So in this case also the content inside the reactor is continuously mixed. So the system which is homogeneity inside the reactor, so this reactor we call back mixing reactors so that means the concentration or the conversion at any locations at a particular time is constant. Whereas, in case of ideal plug flow reactor it is a tubular kind of reactor where the flow enters in one end and it exits to the other.

And there is no back mixing that means there is no axial mixing. So all the contents are radially mixing at any locations, but they are not back mixed. So, let us consider this is a plug flow reactor and we have a feed in F_{j0} and feed product exit at a molar flow rate of F_j that is exit and this is in. Now, if we consider a very small elements, say this is Δy and the location over here is say y and at this location it is $y + \Delta y$.

So, if we take this control volume, so the inlet to this control volume say delta v is the control volume and inlet to this is of component J is Fj(y) and exit from here is Fj($y + \Delta y$). So now we need to divide the reactor into number of sub-volumes like this. So it can be divided into number of sub-volumes. And within the sub-volume that is delta v which is written over here this sub-volume the reaction rate may consider spatially uniform.

As you can see, since there is no back mixing in this reactor when the reaction will proceed the rate will change that means the rate is not spatially constant throughout the length of the reactor. But if we divide the reactor with a into a number of small sub-volumes and then for each sub-volumes we assume that the reaction rate is spatially uniform.

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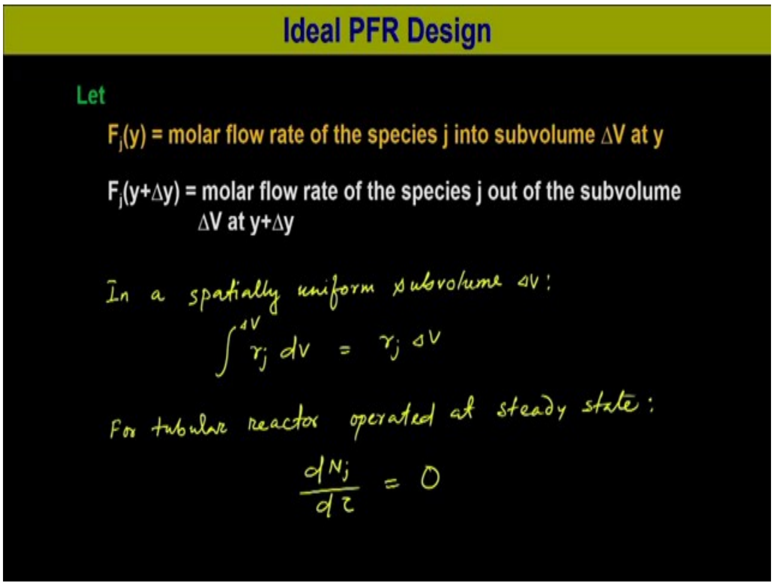

Ideal PFR Design

Let

$F_j(y)$ = molar flow rate of the species j into subvolume ΔV at y

$F_j(y+\Delta y)$ = molar flow rate of the species j out of the subvolume ΔV at $y+\Delta y$

In a spatially uniform subvolume ΔV:

$$\int^{\Delta V} r_j \, dV = r_j \Delta V$$

For tubular reactor operated at steady state:

$$\frac{dN_j}{d\tau} = 0$$

Now, let consider

Fj(y) = molar flow rate of species j into sub-volumes ΔV at y, and

Fj($y + \Delta y$) = molar flow rate of the species j out of the sub-volume that is ΔV at $y + \Delta y$.

That we have assumed. Now in a spatially uniform sub-volume we can write

$$\int^{\Delta V} r_j dV = r_j \Delta V$$

So we can takeout from the integral because we assume for the small sub-volumes, the rate is spatially uniform. Now, for tubular reactor if it operates at steady state for tubular reactor, operated at steady state

$$\frac{dN_j}{d\tau} = 0\ 7$$

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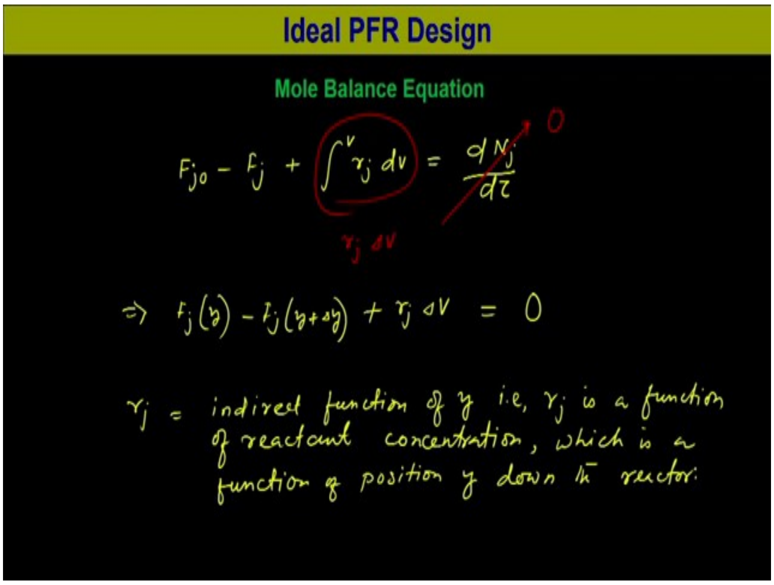

Ideal PFR Design

Mole Balance Equation

$$F_{j0} - F_j + \boxed{\int^{V} r_j\, dV} = \cancel{\frac{dN_j}{d\tau}} \to 0$$

$r_j\, \Delta V$

$$\Rightarrow F_j(y) - F_j(y+\Delta y) + r_j\, \Delta V = 0$$

r_j = indirect function of y i.e, r_j is a function of reactant concentration, which is a function of position y down the reactor.

So using these two equation if we apply in the general mole balance equation we can obtain the mole balance equations we know which is

$$F_{j0} - F_j + \int^{V} r_j dV = \frac{dN_j}{d\tau}$$

So this part, this is 0 at steady state, and this part is $r_j \Delta V$. So we can write from here

$$F_j(y) - F_j(y + \Delta y) + r_j \Delta V = 0$$

Here r_j is the indirect function of y that is r_j is a function of reactant and concentration. So then reactant concentration is a function of y down the reactors. So the reactant concentration, which is a function of position y down the reactor.

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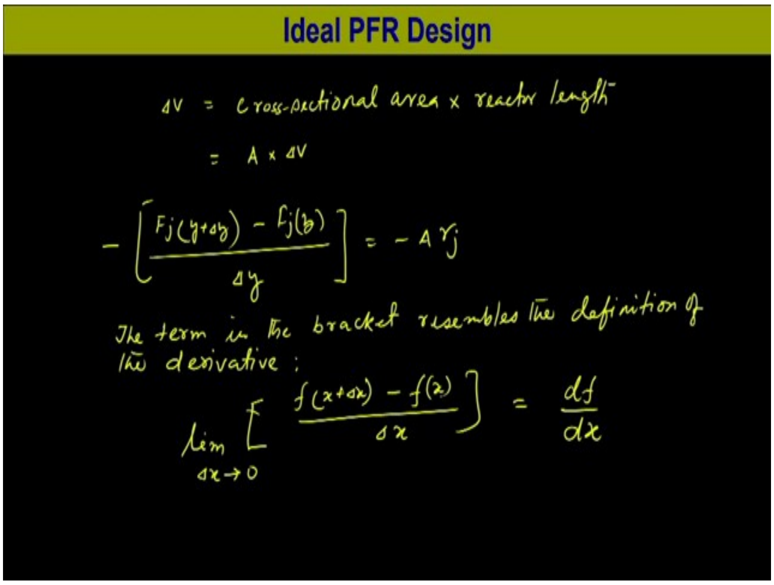

Ideal PFR Design

ΔV = cross-sectional area × reactor length

= $A \times \Delta V$

$$-\left[\frac{F_j(y+\Delta y) - F_j(y)}{\Delta y}\right] = -A r_j$$

The term in the bracket resembles the definition of the derivative :

$$\lim_{\Delta x \to 0}\left[\frac{f(x+\Delta x) - f(x)}{\Delta x}\right] = \frac{df}{dx}$$

Now, if we take ΔV as we consider is the cross sectional area we can write this one would be cross sectional area into the reactor length. So if we take the control volume the cross sectional area is $A * \Delta V$. So we can write the earlier equation which you have derived is

$$-\left[\frac{F_j(y+\Delta y) - F_j(y)}{\Delta y}\right] = -A r_j$$

So the term in that bracket resembles the definition of derivative, then we can write

$$\lim_{\Delta x \to 0}\left[\frac{f_j(\mathrm{x}+\Delta x) - f_j(\mathrm{x})}{\Delta x}\right] = \frac{df}{dx}$$

So this is the definition so the term over here in the bracket is also the definition of this derivative.

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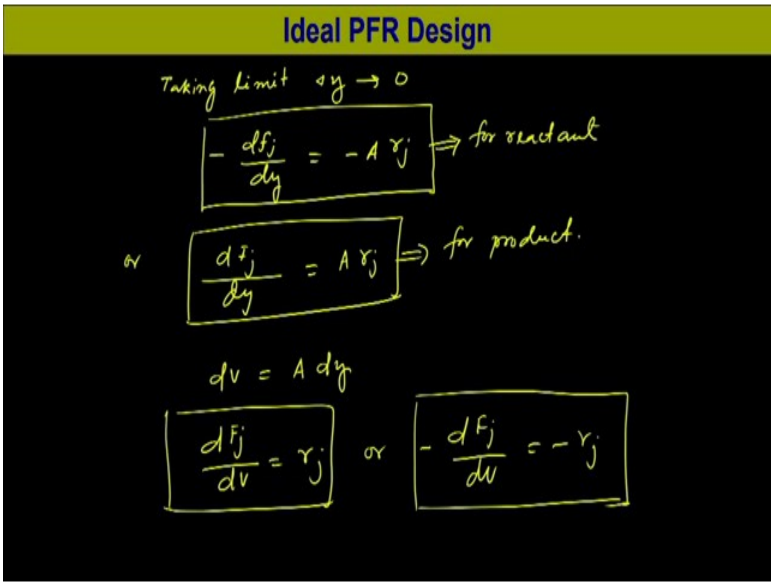

Ideal PFR Design

Taking Limit $\Delta y \to 0$

$$\boxed{-\frac{df_j}{dy} = -A r_j} \Rightarrow \text{for reactant}$$

or

$$\boxed{\frac{dF_j}{dy} = A r_j} \Rightarrow \text{for product.}$$

$$dV = A\,dy$$

$$\boxed{\frac{dF_j}{dV} = r_j} \quad \text{or} \quad \boxed{-\frac{dF_j}{dV} = -r_j}$$

So, we can write taking limit Δy tends to 0 it would come

$$-\frac{df_j}{dx} = -Ar_j$$

So this is for the reactant. For the product we can write

$$\frac{dF_j}{dx} = Ar_j$$

So this is for the product. But it is generally more convenient to write this balance equation in terms of the reactor volume instead of the reactor length y. So if we convert length to volume we can write

$$dV = Ady$$

So, if we substitute this over here we will get

$$\frac{dF_j}{dV} = r_j$$

or

$$-\frac{dF_j}{dV} = -r_j$$

So these are the two forms, this is for the product and this for the reactant in terms of the volume.

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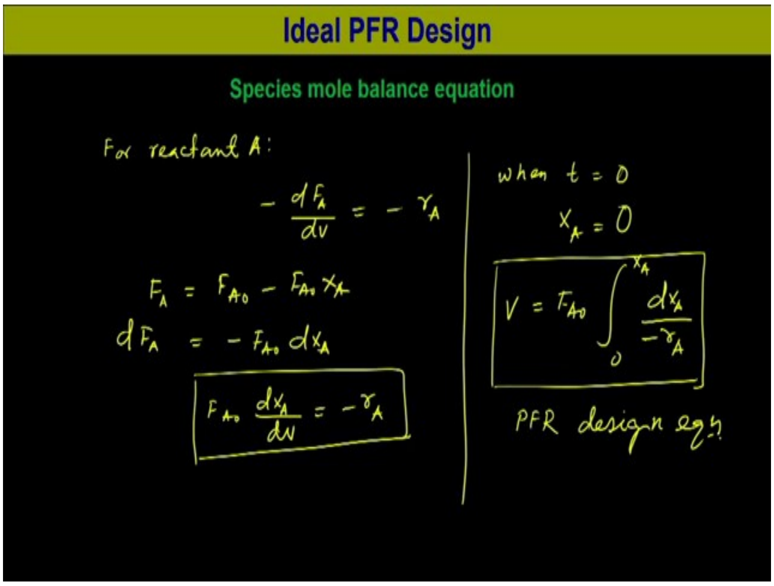

Ideal PFR Design

Species mole balance equation

For reactant A:

$$-\frac{dF_A}{dV} = -r_A$$

$$F_A = F_{A0} - F_{A0}X_A$$

$$dF_A = -F_{A0}\,dX_A$$

$$\boxed{F_{A0}\frac{dX_A}{dV} = -r_A}$$

when $t = 0$

$X_A = 0$

$$\boxed{V = F_{A0}\int_0^{X_A}\frac{dX_A}{-r_A}}$$

PFR design eqn

Now, if we write this balance equation for a particular species A. So the species mole balance for component A. The mole balance equation would be

$$-\frac{dF_A}{dV} = -r_A$$

Now, we know that F_A for a single reactions

$$F_A = F_{A0} - F_{A0}X_A$$

and dF_A if we just differentiate,

$$dF_A = -F_{A0}dX_A$$

So from here we can write,

$$F_{A0}\frac{dX_A}{dV} = -r_A$$

Now, if we apply the conditions when t = 0, X_A = 0. So if we integrate this equations it would give

$$V = F_{A0}\int_0^{X_A}\frac{dX_A}{-r_A}$$

So this is the well-known PFR, Plug Flow Reactor design equation.

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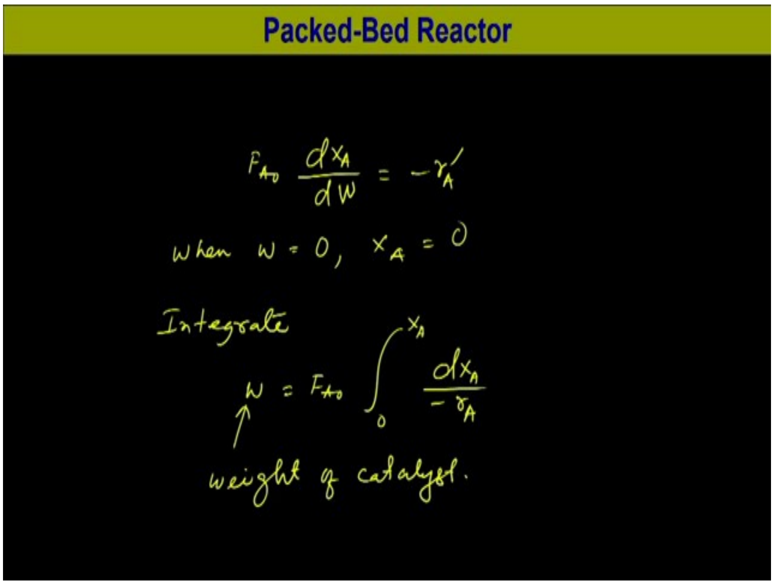

Packed-Bed Reactor

$$F_{A0}\frac{dx_A}{dW} = -r_A'$$

when $W = 0$, $x_A = 0$

Integrate

$$W = F_{A0}\int_0^{x_A}\frac{dx_A}{-r_A}$$

↑

weight of catalyst.

If we consider Packed Bed Reactor. The derivation of the integral and the differential form of the design equation for Packed Bed Reactor is similar to the Plug Flow Reactor. So in this case we can write

$$F_{A0}\frac{dX_A}{dw} = -r_A^{'}$$

So in this case instead of the volume of the reactor we just replaced with the weight of the catalyst, so which would be equal to $-r_A^{'}$. When we have t = 0, X_A = 0. Initially then we can integrate this. So if we integrate, we will obtain

$$w = F_{A0}\int_0^{X_A}\frac{dX_A}{-r_A^{'}}$$

here w is the weight of catalyst.

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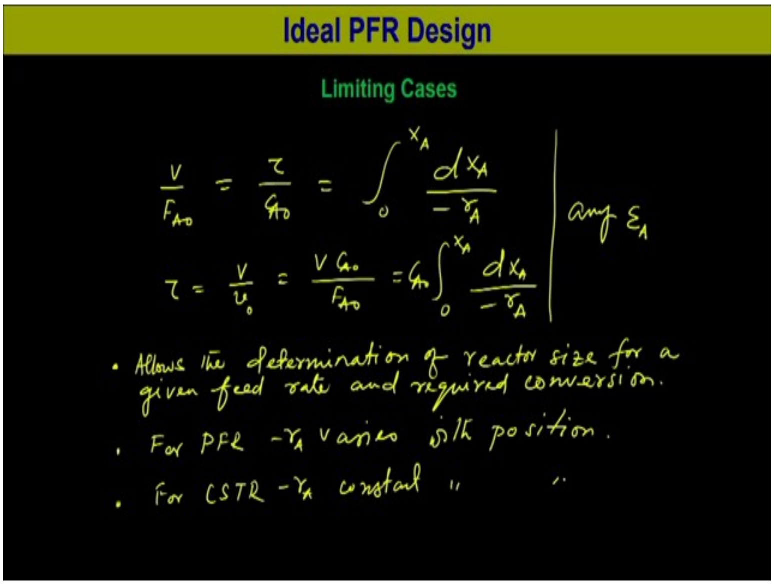

Ideal PFR Design

Limiting Cases

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = \frac{V C_{A0}}{F_{A0}} = C_{A0}\int_0^{X_A} \frac{dX_A}{-r_A}$$

any ε_A

- Allows the determination of reactor size for a given feed rate and required conversion.
- For PFR $-r_A$ varies with position.
- For CSTR $-r_A$ constant " ".

Now, if we return back to the Plug Flow Reactor design, we can see two limiting cases, in one case for any epsilon or any varying volume system the design equation would be

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

and we can write

$$\tau = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A}$$

So these two relations is valid for any ε_A and this allows the determination of the reactor size for a given feed rate and required conversion. So if we have the feed rate given over here and then if the conversion is mentioned so for a particular kinetics we can calculate the size of the reactor required. As we can see for Plug Flow Reactor this $-r_A$ varies with position. However, in case of CSTR or mixed flow reactor $-r_A$ is constant with position.

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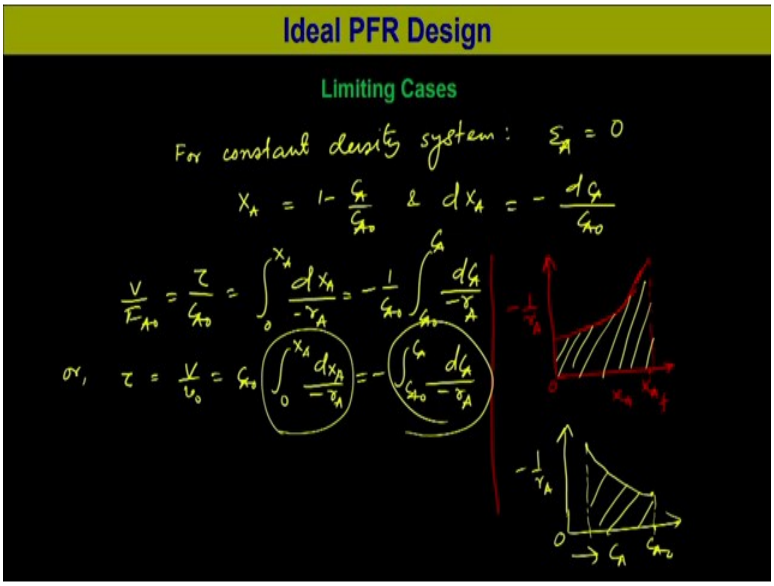

Ideal PFR Design

Limiting Cases

For constant density system: $\varepsilon_A = 0$

$X_A = 1 - \frac{C_A}{C_{A0}}$ & $dX_A = -\frac{dC_A}{C_{A0}}$

$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}} \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$

or, $\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_A} \frac{dx_A}{-r_A} = -\int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$

Now, if we consider the constant density system in that case, $\varepsilon_A = 0$, and we can write, we know that

$$X_A = 1 - \frac{C_A}{C_{A0}}$$

and then we can write

$$dX_A = -\frac{dC_A}{C_{A0}}$$

So in this case the performance equation

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}} \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

So, or we can write

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$$

In terms of concentration we can write

$$= -\int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

Now, if we look into the graphical representation of $-r_A$ versus conversion or $-\frac{1}{r_A}$ versus concentration change it would look like this. So this is $-\frac{1}{r_A}$ versus conversion X_A. Say it start from 0 and say conversion is X_{Af}.

So the rate will be, so this is the area under the curve so the conversion for 0 to X_A will take this volume. So from this area we can calculate the area under the curve. So integral 0 to X_A $\frac{dX_A}{-r_A}$. So this term we can calculate from this. Similarly, if we plot $-\frac{1}{r_A}$ versus C_A concentration. So this is 0 and this at C_{A0}, so $-\frac{1}{r_A}$ will be increase because the rate is decreased. So this is how we can calculate this area under this curve.

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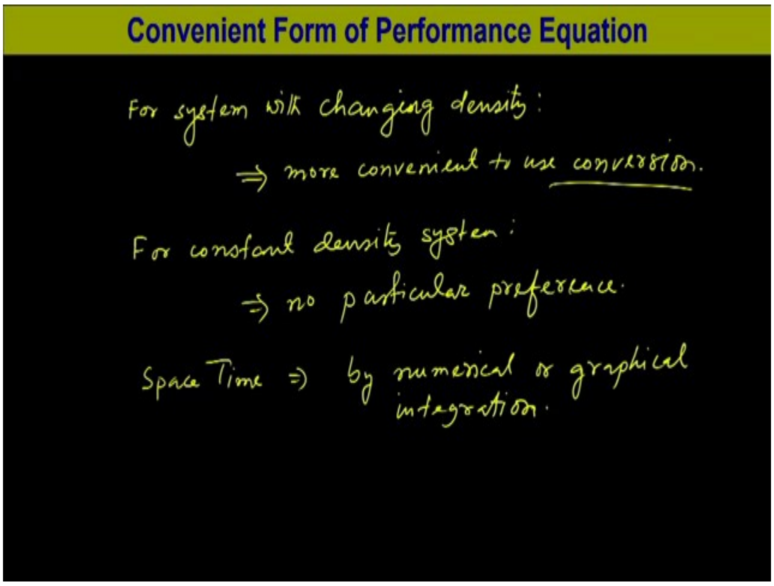

Convenient Form of Performance Equation

For system with changing density:

⇒ more convenient to use conversion.

For constant density system:

⇒ no particular preference.

Space Time ⇒ by numerical or graphical integration.

Now, the performance equation can be written in the convenient form, we can write in terms of the concentration or we can write in terms of the conversion. For system with changing density, the more convenient form is, more convenient to use conversion but for constant density system, no particular preference. So this are the convenient form which we can have the changing density system.

So the more convenient form would be conversion, but for constant density system there is no particular preference so either we can use the concentration form or performance equation in terms of the concentration or we can use in terms of the conversion. The space time which is required for any particular duty can be obtained the space time can be obtained either by numerical or graphical integration. However, for certain simple kinetics analytical integration is also possible.

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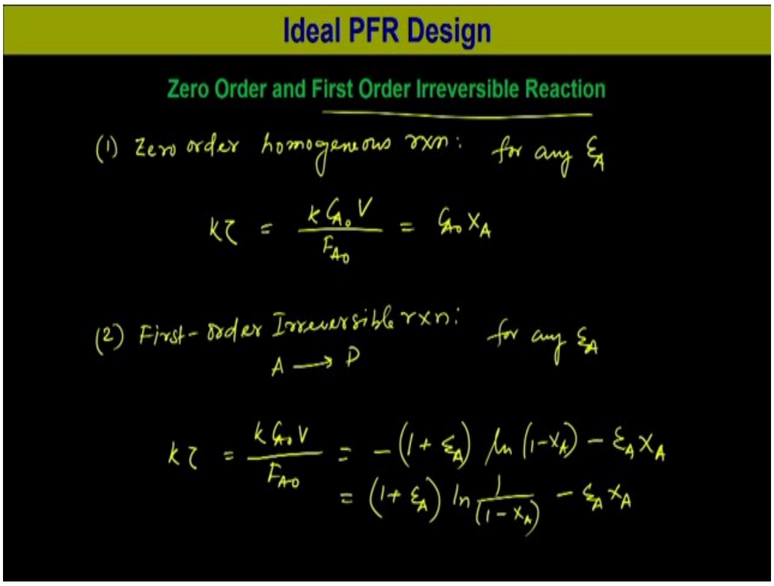

Ideal PFR Design

Zero Order and First Order Irreversible Reaction

(1) Zero order homogeneous rxn: for any ε_A

$$k\tau = \frac{kC_{A0}V}{F_{A0}} = C_{A0}X_A$$

(2) First-order Irreversible rxn: for any ε_A

A → P

$$k\tau = \frac{kC_{A0}V}{F_{A0}} = -(1+\varepsilon_A)\ln(1-X_A) - \varepsilon_A X_A$$

$$= (1+\varepsilon_A)\ln\frac{1}{(1-X_A)} - \varepsilon_A X_A$$

Let us consider some different kind of reactions and see analytically how we can calculate the space time for a particular duty. If we consider 0 order homogeneous reaction for any ε_A. We can write

$$k\tau = \frac{kVC_{A0}}{F_{A0}} = C_{A0}X_A$$

For first order irreversible reaction, so if we consider first order irreversible reaction say

$$A \to product$$

And for any ε_A we can write

$$k\tau = \frac{kVC_{A0}}{F_{A0}} = -(1+\varepsilon_A)\ln(1-X_A) - \varepsilon_A X_A$$

This we can rearrange at

$$= (1+\varepsilon_A)\ln\frac{1}{(1-X_A)} - \varepsilon_A X_A$$

So this is for first order irreversible reaction and this is for 0 order homogeneous reaction.

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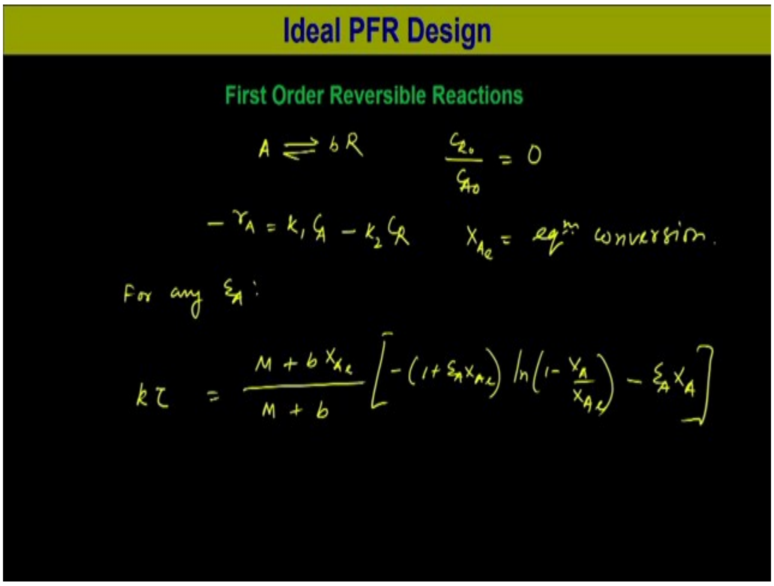

Ideal PFR Design

First Order Reversible Reactions

$A \rightleftharpoons bR \qquad \frac{C_{R0}}{C_{A0}} = 0$

$-r_A = k_1 C_A - k_2 C_R \qquad X_{Ae} =$ eq^m conversion.

For any ε_A:

$$k\tau = \frac{M + bX_{Ae}}{M+b}\left[-(1+\varepsilon_A X_{Ae})\ln\left(1-\frac{X_A}{X_{Ae}}\right) - \varepsilon_A X_A\right]$$

Now, if we consider first order reversible reaction, so first order reversible reaction say consider

$$A \rightleftharpoons bR$$

$$\frac{C_{R0}}{C_{A0}} = 0$$

and the kinetics is

$$-r_A = k_1 C_A - k_2 C_R$$

and the equilibrium conversion X_{Ae} this is the equilibrium conversion. So we can write for any ε_A we can write

$$k\tau = \frac{M + bX_{Ae}}{M+b}\left[-(1+\varepsilon_A)\ln(1-X_A) - \varepsilon_A X_A\right]$$

So this is for first order reversible reaction.

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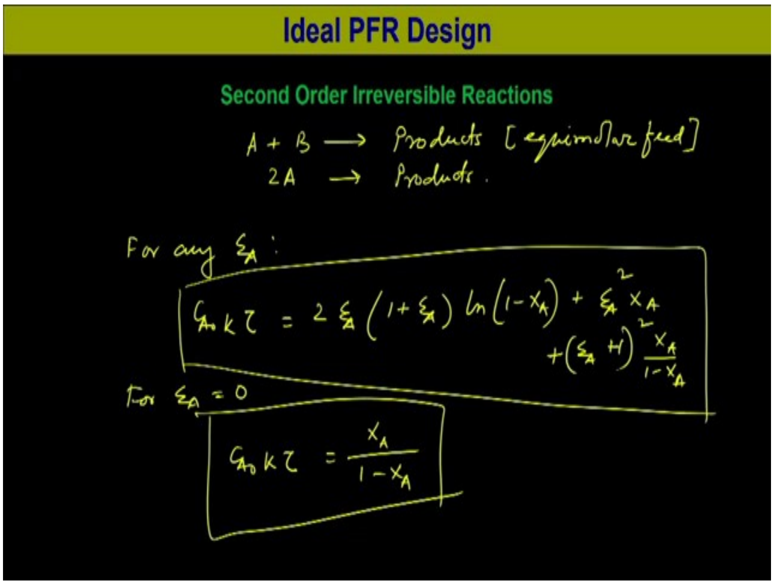

Ideal PFR Design

Second Order Irreversible Reactions

$A + B \longrightarrow$ Products [equimolar feed]

$2A \longrightarrow$ Products.

For any ε_A :

$$\boxed{C_{A0} k \tau = 2\varepsilon_A (1+\varepsilon_A) \ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1-X_A}}$$

For $\varepsilon_A = 0$

$$\boxed{C_{A0} k \tau = \frac{X_A}{1-X_A}}$$

Similarly, we can also derive the integral form if we just integrate we will get a convenient form of second order irreversible reaction. Say if we consider

$$A + B \rightarrow products$$
$$2A \rightarrow products$$

This is for this case assume equimolar feed. Now for any ε_A we can write get

$$C_{A0}k\tau = 2\varepsilon_A(1+\varepsilon_A)\ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1-X_A}$$

Now, if we write this for $\varepsilon_A = 0$ we can put over here so this term will cancel out and this term will cancel out. So we will have $\frac{X_A}{1-X_A}$. So we will get the simplified form

$$C_{A0}k\tau = \frac{X_A}{1-X_A}$$

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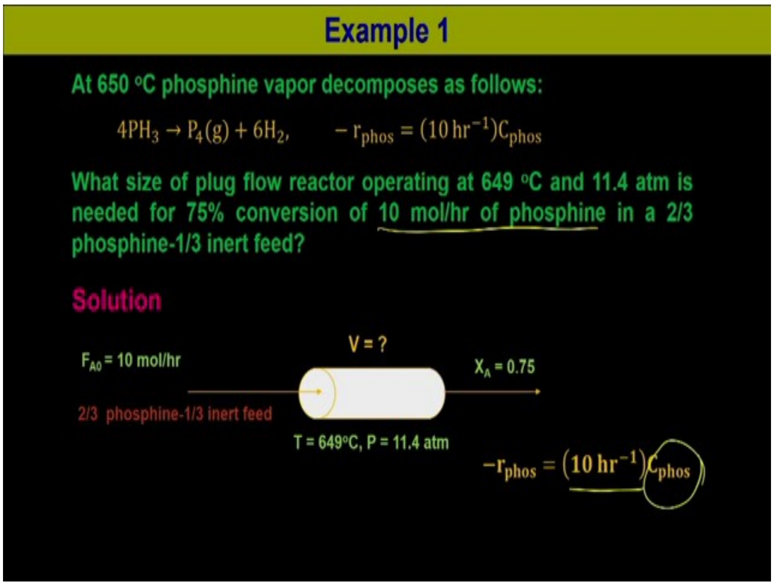

Example 1

At 650 °C phosphine vapor decomposes as follows:

$$4PH_3 \rightarrow P_4(g) + 6H_2, \qquad -r_{phos} = (10\,hr^{-1})C_{phos}$$

What size of plug flow reactor operating at 649 °C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine-1/3 inert feed?

Solution

F_{A0} = 10 mol/hr

2/3 phosphine-1/3 inert feed

V = ?

X_A = 0.75

T = 649°C, P = 11.4 atm

$-r_{phos} = (10\,hr^{-1})C_{phos}$

Now, let us take an example to see how to calculate the volume of the reactor for a particular operation or particular job. So at 650 degree centigrade phosphine vapour decomposes as follows, phase forms

$$4PH_3 \rightarrow P_4(g) + 6H_2O$$

with the rate of reactions $-r_{phos} = (10hr^{-1})C_{phos}$. Now we need to calculate what size of plug flow reactor operating at 649 degree centigrade and 11.4 atmosphere is needed for 75 percent conversion of 10 (molar) mole per hour of phosphine in a two third phosphine and one third inert feed.

So the feed is, feed flow rate is 10 mole per hour of phosphine and the phosphine and inert composition is two third and one third in the feed. Now we need to find out the size of the plug flow reactor needed which is for the conversion of 75 percent. Now let us solve it, this is our plug flow reactor and we have molar flow rate of the phosphine in the feed is 10 mole per hour. Please note that this 10 mole per hour of the phosphine is the phosphine feed rate phosphine in the feed.

But the total feed which also includes the inert that also has not been included in F_{A0}, F_{A0} is basically the amount of phosphine which is in the feed. Now, two third phosphine and one third inert feed. The conversion is 0.75 temperature and pressure condition is given T is equal to 649 degree centigrade and P is equal to 11.4 atmosphere these are the total pressure and temperature conditions.

We need to, we have given the rate of the reactions which is given the rate equations and we can see from the rate equations this is first order. So this is first order reaction because it is the proportional the rate is proportional to the concentration of the phosphine. So we need to find out the volume of the reactor needed.

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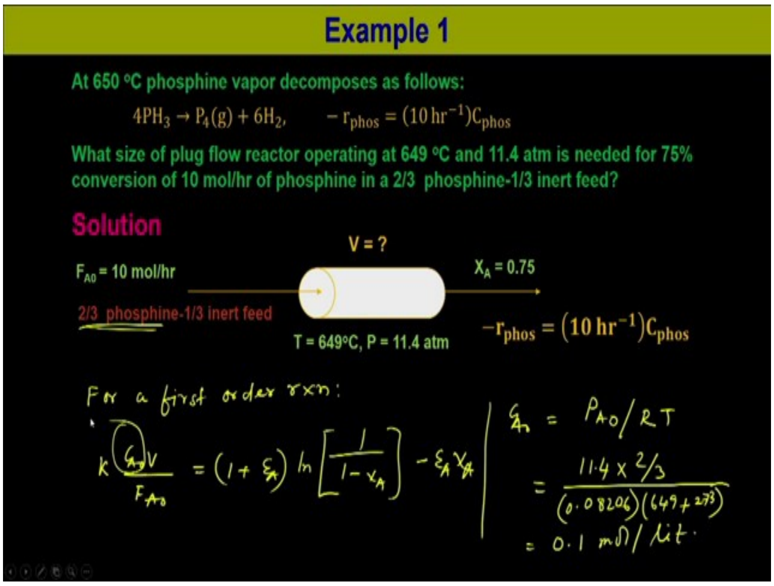

Example 1

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What size of plug flow reactor operating at 649 °C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine-1/3 inert feed?

Solution

For a first order rxn:

$$\frac{k\,C_{A0}V}{F_{A0}} = (1+\varepsilon_A)\ln\left[\frac{1}{1-X_A}\right] - \varepsilon_A X_A$$

$$C_{A0} = P_{A0}/RT = \frac{11.4 \times 2/3}{(0.08206)(649+273)} = 0.1\ mol/lit.$$

Now this is our, so for first order reaction we know that

$$\frac{kVC_{A0}}{F_{A0}} = (1+\varepsilon_A)\ln\left[\frac{1}{1-X_A}\right] - \varepsilon_A X_A$$

So this is the equations so we have to find out the conversion is given we have to find out C_{A0} from the conditions which are given. So if you find out C_{A0} we can write

$$C_{A0} = \frac{P_{A0}}{RT}$$

Now P_{A0} would be the total pressure is 11.4 atmosphere and per cell pressure of phosphine would be two third. So this is

$$= \frac{11.4 * 2/3}{(0.08206)(649+273)}$$

So if we calculate it would give 0.1 mole per litter. So now we have calculated C_{A0}.

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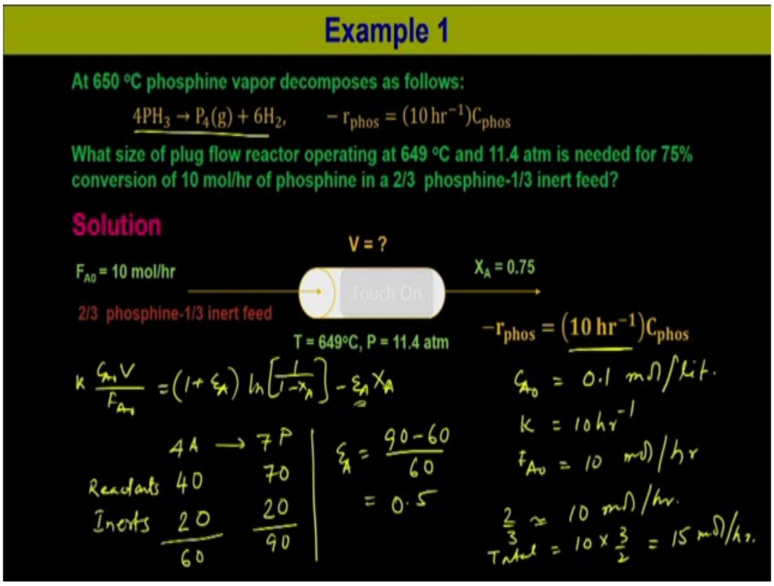

Example 1

At 650 °C phosphine vapor decomposes as follows:

$4PH_3 \rightarrow P_4(g) + 6H_2$, $\quad -r_{phos} = (10\,hr^{-1})C_{phos}$

What size of plug flow reactor operating at 649 °C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine-1/3 inert feed?

Solution

$V = ?$

F_{A0} = 10 mol/hr

2/3 phosphine-1/3 inert feed

$X_A = 0.75$

T = 649°C, P = 11.4 atm

$-r_{phos} = (10\,hr^{-1})C_{phos}$

$$k\frac{C_{A0}V}{F_{A0}} = (1+\varepsilon_A)\ln\left[\frac{1}{1-X_A}\right] - \varepsilon_A X_A$$

$$\begin{array}{lcc} & 4A \longrightarrow & 7P \\ \text{Reactants} & 40 & 70 \\ \text{Inerts} & 20 & 20 \\ \hline & 60 & 90 \end{array}$$

$$\varepsilon_A = \frac{90-60}{60} = 0.5$$

C_{A0} = 0.1 mol/lit.

k = 10 hr^{-1}

F_{A0} = 10 mol/hr

$\frac{2}{3} \approx$ 10 mol/hr.

Total = $10 \times \frac{3}{2}$ = 15 mol/hr.

So our equation is

$$\frac{kVC_{A0}}{F_{A0}} = (1+\varepsilon_A)\ln\left[\frac{1}{1-X_A}\right] - \varepsilon_A X_A$$

so we have calculated C_{A0} which is 0.1 mole per liter. Now k is given from this relation k is 10 hour^{-1}, F_{A0} is also given is 10 mole per hour. Now we have to calculate ε_A. If we look into the reaction here it is forming 4 mole of reactant forming 7 mole of product.

So the reactant we had 10 mole per hour phosphine. So we had reactant this is 4 times 40 moles will produce 70 and inerts. So two third is equivalent to 10 mole per hour, so total is equal to

$$10 * \frac{3}{2} = 15 mol/hr$$

So our inert contain in a initially is about is 5 mole per hour. So if we take 4 times of that volume, so 5*4 so inert is 20 so it would present it will remains same after the reaction each over.

So it would be 20, so if just sum them up it will be 90 and this will be 60. So now if we calculate

$$\varepsilon_A = \frac{90-60}{60}$$

So this would be 0.5. So now we have ε_A, F_{A0}, C_{A0}, k and conversion is 0.75.

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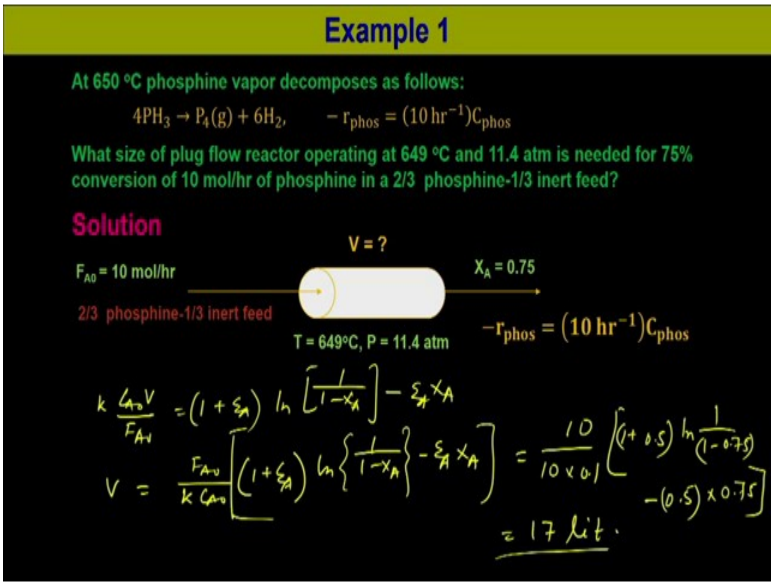

Example 1

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What size of plug flow reactor operating at 649 °C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine-1/3 inert feed?

Solution

$$k\frac{C_{A0}V}{F_{A0}} = (1+\varepsilon_A)\ln\left[\frac{1}{1-X_A}\right] - \varepsilon_A X_A$$

$$V = \frac{F_{A0}}{kC_{A0}}\left[(1+\varepsilon_A)\ln\left\{\frac{1}{1-X_A}\right\} - \varepsilon_A X_A\right] = \frac{10}{10\times 0.1}\left[(1+0.5)\ln\frac{1}{(1-0.75)} - (0.5)\times 0.75\right]$$

$$= \underline{17\ lit.}$$

Now, if we substitute these values in the equation so

$$\frac{kVC_{A0}}{F_{A0}} = (1+\varepsilon_A)\ln\left[\frac{1}{1-X_A}\right] - \varepsilon_A X_A$$

Now if we substitute the values the v would be equal to, so if we rearrange this equation

$$k = \frac{F_{A0}}{VC_{A0}}\left[(1+\varepsilon_A)\ln\left\{\frac{1}{1-X_A}\right\} - \varepsilon_A X_A\right]$$

Now if you substitute

$$k = \frac{10}{10*0.1}\left[(1+0.5)\ln\left\{\frac{1}{1-0.75}\right\} - 0.5*0.75\right]$$

So this would give 17 liter. So the volume of the reactor needed for this particular reactions to happen for 70 for conversion would require 17 litter.

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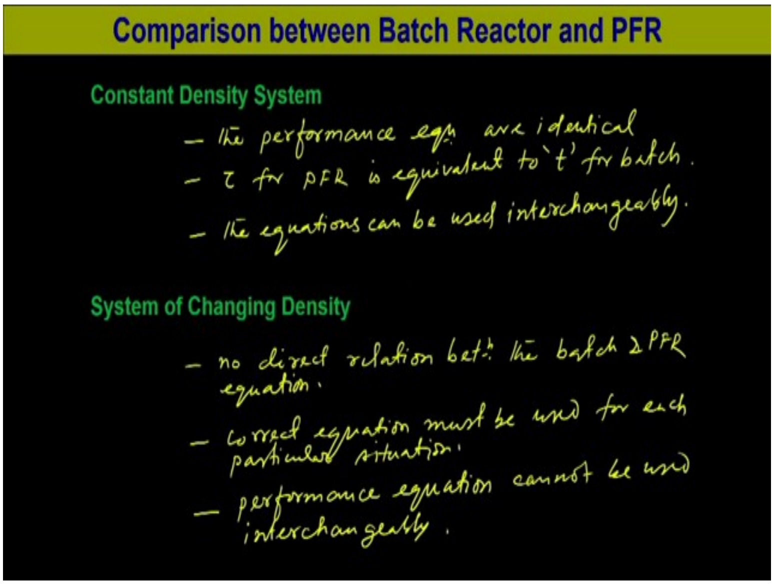

Comparison between Batch Reactor and PFR

Constant Density System

- the performance eq^n are identical
- τ for PFR is equivalent to 't' for batch.
- the equations can be used interchangeably.

System of Changing Density

- no direct relation bet^n the batch & PFR equation.
- correct equation must be used for each particular situation.
- performance equation cannot be used interchangeably.

So now, if we look into the, if we compare between the batch reactor and plug flow reactor we can see that for constant density system the performance equation for batch reactor and plug flow reactor are identical. So the performance equation are identical τ for PFR is equivalent to 't' for batch, 't' for batch reactor. The equations can be used interchangeably. Now, if it is variable density system in that case there is no direct relations between the batch reactor and the plug flow reactor.

So, no direct relation between the batch and PFR equation. So the correct equation must be used for each particular situation and the performance equation cannot be used interchangeably. As we can see only for constant density system there is direct relations between the batch reactor and the plug flow reactor, but in case of the changing density system there is no direct co-relations among them and appropriate care has to be taken while using or solving some problem.

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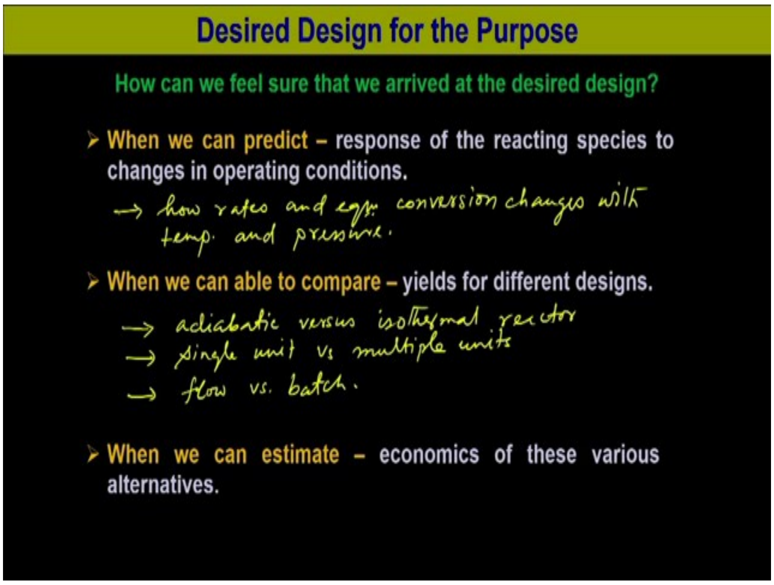

Desired Design for the Purpose

How can we feel sure that we arrived at the desired design?

- **When we can predict** – response of the reacting species to changes in operating conditions.
  - → how rates and eqm. conversion changes with temp. and pressure.
- **When we can able to compare** – yields for different designs.
  - → adiabatic versus isothermal reactor
  - → single unit vs multiple units
  - → flow vs. batch.
- **When we can estimate** – economics of these various alternatives.

Now, for desired design for the purpose how can we feel sure that we arrived at the desired design equation? This can be, we can feel sure when we can predict the response of the reacting species to changes in the operating conditions. That means how rates and equilibrium conversion changes with temperature and pressure. So if we can predict how rates and equilibrium and conversion changes with temperature and pressure, then we can think that we have arrived to a certain design.

But also same time when we can able to compare yields for different designs like adiabatic versus isothermal reactor. Secondly single unit versus multiple unit and third is flow versus batch. So if we are able to compare the yields for different design, if we have adiabatic system and isothermal reactor, how their yields changes if we can compare or if we use single reactor what would be the yield and instead of multiple reactors or whether we can compare the yields among the flow and batch reactor.

And finally, if we can estimate the economics of these various alternatives. So, if we can make sure that the economics as per the requirements of the yields and the changing parameters like conversion with temperature and pressure if we are feel sure then finally we estimate the economics of the various alternatives, then only we can feel sure that we arrived at the desired design. So for a particular design we need to care for all of these steps.

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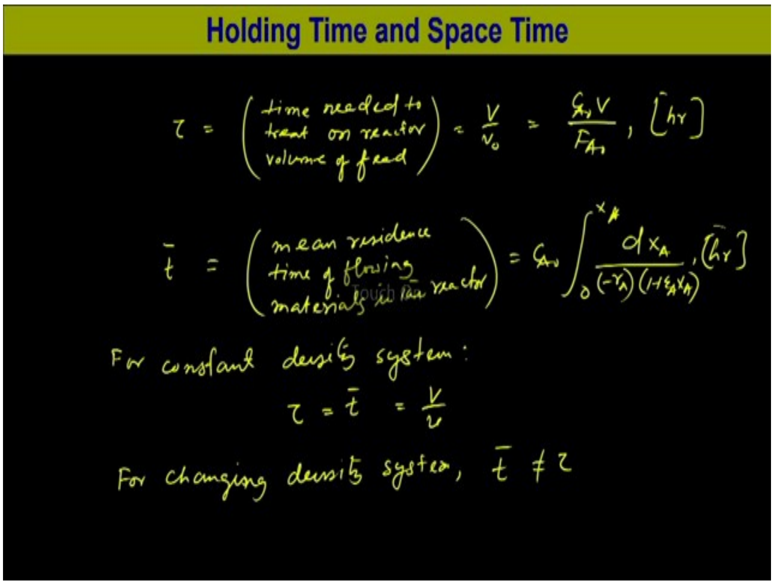

Holding Time and Space Time

$$\tau = \begin{pmatrix}\text{time needed to}\\ \text{treat on reactor}\\ \text{volume of feed}\end{pmatrix} = \frac{V}{v_0} = \frac{C_{A0}V}{F_{A0}}, \ [hr]$$

$$\bar{t} = \begin{pmatrix}\text{mean residence}\\ \text{time of flowing}\\ \text{materials in the reactor}\end{pmatrix} = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}, \ [hr]$$

For constant density system:

$$\tau = \bar{t} = \frac{V}{v}$$

For changing density system, $\bar{t} \neq \tau$

Now two things, one is holding time and the space time. Space time we have already discussed earlier which we have defined τ is equal to time needed to treat on reactor volume of feed at specified condition which is

$$\tau = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}}$$

And the unit is time, $\bar{t}$ is the mean residence time of flowing materials in the reactor. This is nothing but

$$\bar{t} = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}$$

and the unit is also time.

If it is constant density system the both space time and holding time they are same. So for constant density system τ is equal to $\bar{t}$ which is equal to v by volumetric fluid, but for changing density system $\bar{t}$ is not equal to τ .

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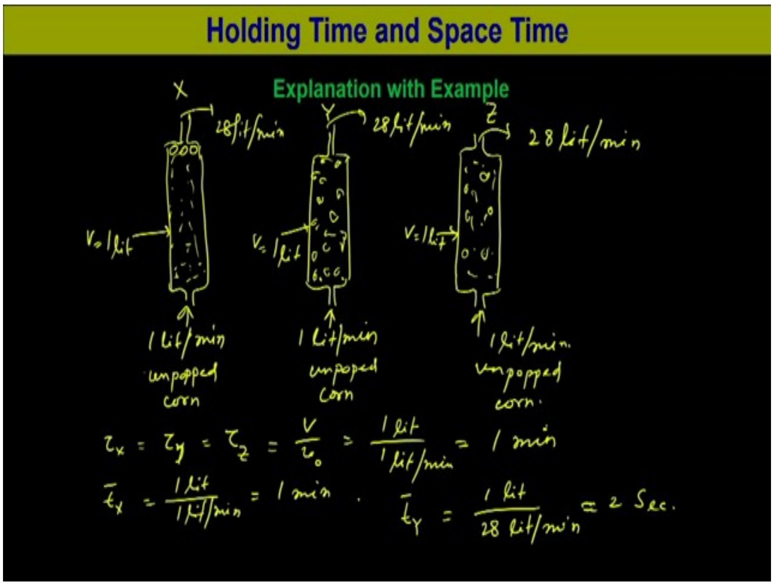

Holding Time and Space Time

Explanation with Example

$$\tau_x = \tau_y = \tau_z = \frac{V}{v_o} = \frac{1\ lit}{1\ lit/min} = 1\ min$$

$$\bar{t}_x = \frac{1\ lit}{1\ lit/min} = 1\ min . \quad \bar{t}_Y = \frac{1\ lit}{28\ lit/min} \simeq 2\ Sec.$$

Let us take a very good example given in Levienspiel and in this case it is consider a popping up of the popcorn. So 3 cases have been considered, 3 same reactor size have been taken and the volume is same V is equal to 1 litter and un-popped popcorn is fed at the bottom at 1 litter per minute this is also 1 litter per minute. This is un-popped corn and the corn are taken inside and for the first case say X, Y, and Z the product rate is given to a 28 litter per minute.

So in the first case, the case X the popping of, so for the product rate is same for both the, all the cases 28 litter per minute, the popping up happens at the top of the reactor, but in case of second case the popping up occurs at the bottom of the reactors. So the residence time for the second case and in the third case it is happened intermittently. So if we look into the different values that is

$$\tau_X = \tau_Y = \tau_Z = \frac{V}{v_0} = \frac{1 lit}{1 lit / \min}$$

So the time is 1 minute, but in the first case when the popping up occurs at the top of the tower, then $\bar{t}_X$ would be equal to 1 litter per, 1 litter per minute which is 1 minute. But in the second case the popping up occurs at the bottom so the popcorn production rate would be same from the bottom to the top so it is 28 litter per minute. So $\bar{t}_Y$ would be equal to 1 litter by 28 litter per minute. So which is equal to 2 second, about 2 second.

So that means in the third case it will varies in between 2 second and 1 minutes. So we can see that the residence time when the popping up occurs at the top is equal to the space time and when the popping up occurs at the bottom of the reactor the residence time decreases because the flow rate increases of the popcorn. So the holding time takes care what happens inside the reactor.

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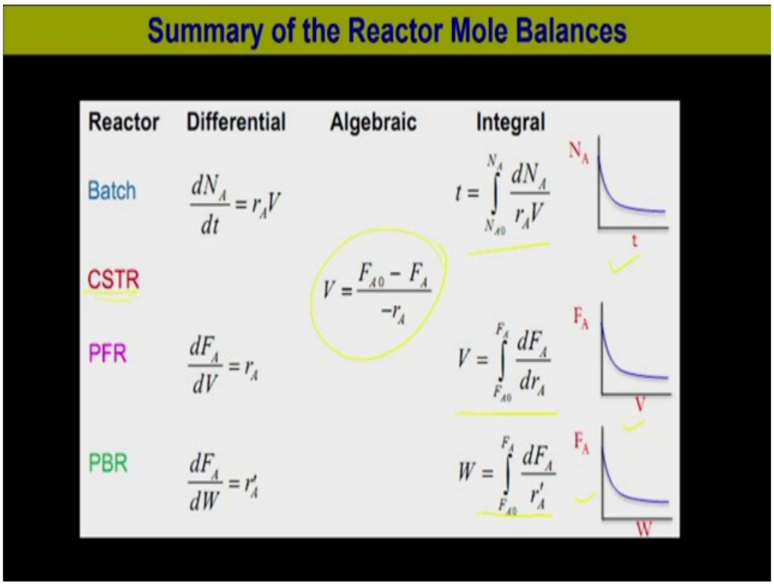

Summary of the Reactor Mole Balances

Reactor	Differential	Algebraic	Integral
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$	
PFR	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{dr_A}$
PBR	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$

Now over all in this 3 lectures we have consider batch, CSTR, Plug Flow and Packed Bed Reactor and these are batch, PFR and packed bed reactor these are differential form, but in case of the CSTR because of the back mixing, so we have only the algebraic form of the equation and then we in case of batch PFR and PBR we can get the integral form of the equation and the profile is look like this.

So this is taken from the Fogler's lecture, I hope you have understood the general mole balance equation for the idealized reactor we have consider. In the next couple of lectures we will consider the reactor design for single reaction, but we will compare the size among the reactors. Thank you for attending this lecture and we will continue our discussion in our next lecture.