Polymer Reaction Engineering
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Lecture-19
Design Equation for Single Reaction System

Welcome to the design equation for single reaction system. In this particular chapter under the head of polymer reaction engineering, we will discuss about the various sections applicable for single reaction system by a mixed flow, mixture reactor, semi batch reactor flow reactor etc. Now, before we go into this particular lecture.

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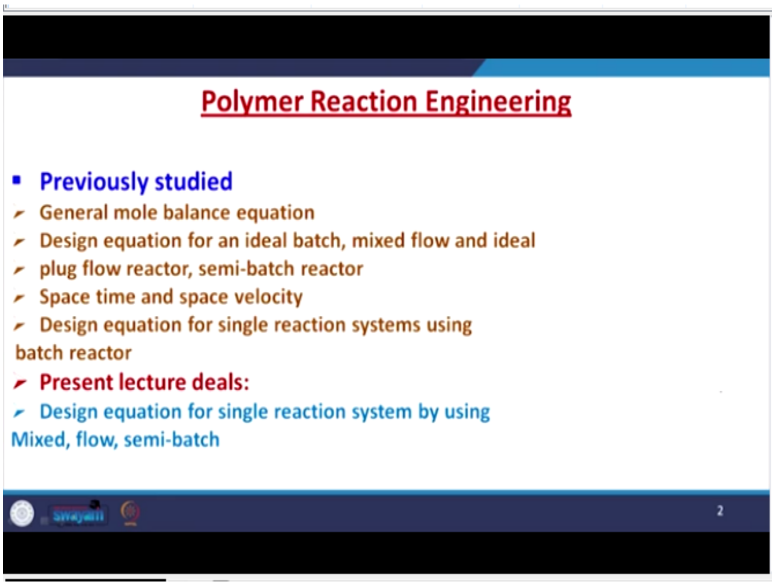

Polymer Reaction Engineering

- Previously studied
- General mole balance equation
- Design equation for an ideal batch, mixed flow and ideal
- plug flow reactor, semi-batch reactor
- Space time and space velocity
- Design equation for single reaction systems using batch reactor
- Present lecture deals:
- Design equation for single reaction system by using Mixed, flow, semi-batch

Just have a brief look at what we had discussed earlier, we described the general mole balance equation, we had a discussion about the general equation for an ideal batch and mix flow reactor, plug flow reactor, semi batch reactor, we had a discussion about the space time and space velocity and what is its significance in the polymer reaction processes. We try to develop the various mathematical equations associated with the single reaction system using the batch reactors.

So, based on this because we have already covered the batch reactor system. In this particular lecture, we are going to discuss about those equations which are applicable for mixed flow and semi batch reactor. Now, let us have a look about various design equations for mixed flow reactor.

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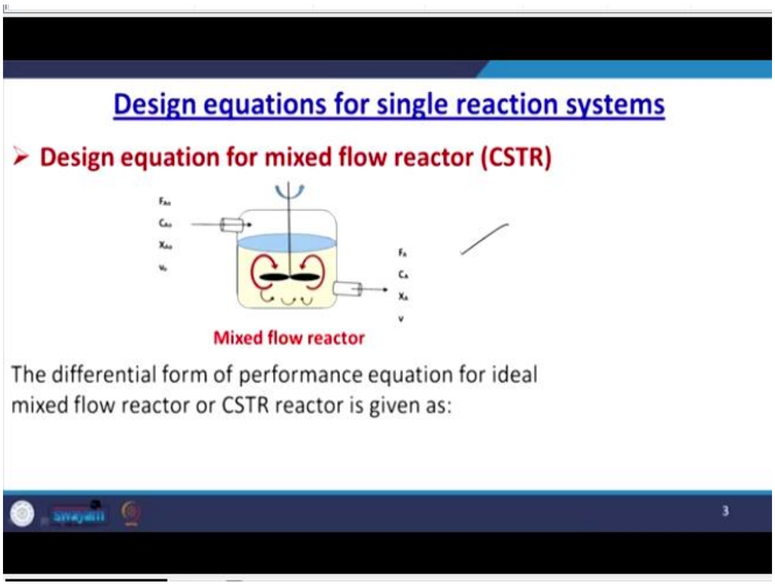

Design equations for single reaction systems

➢ Design equation for mixed flow reactor (CSTR)

Mixed flow reactor

The differential form of performance equation for ideal mixed flow reactor or CSTR reactor is given as:

This is your mix flow reactor if you see that various things are associated, various parameters are closely associated with this particular reactor. Now, if we wish to write the differential form of the performance equation, because performance equation is extremely important for those designing parameter for these polymerization reactions. So, if we would like to describe these performance equations for ideal and explore a CSTR reactor, so, we can write these equations based on the things given over here $F_{i0} - F_i = r_iV$.

So, this is our performance equation for this particular mixed flow reactor. Now, sometimes we need to encounter the single reaction system, the differential equation we need to write for this particular aspect.

The differential form of performance equation for ideal mixed flow reactor or CSTR reactor is given as

$$F_{i_o} - F_i = r_iV$$

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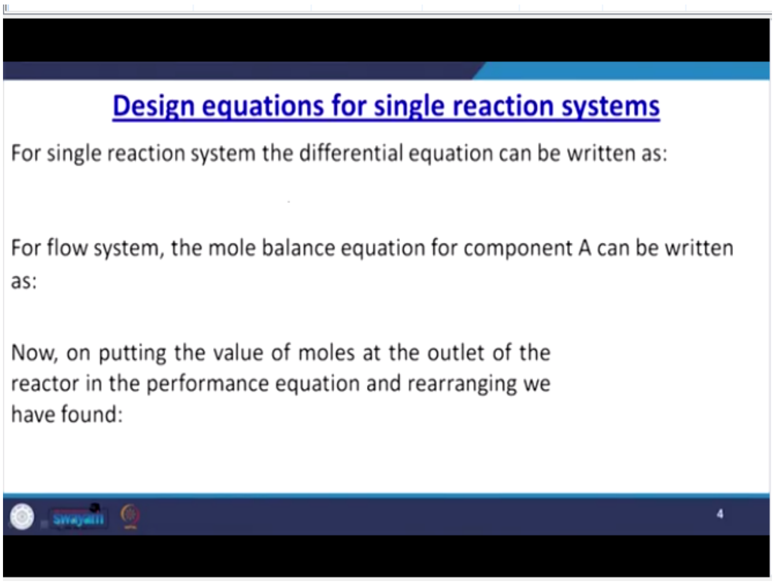

Design equations for single reaction systems

For single reaction system the differential equation can be written as:

For flow system, the mole balance equation for component A can be written as:

Now, on putting the value of moles at the outlet of the reactor in the performance equation and rearranging we have found:

So, it can be written as based on these applicable parameters, which we discussed in this particular figure. This is F_{A0}. So, this is the single reaction system for the differential equation. For single reaction system the above equation can be written as

$$F_{A_o} - F_A = -r_A V$$

Now, sometimes we need to write the mole balance equation for any kind of the component A under the head of a flow system.

For flow system the mole balance equation for any component can be written as

$$F_A = F_{A_o}(1 - X_A)$$

So, these flow system equations can be written as $F_A = F_{A0}(1 - X_A)$ and sometimes referred if you recall the previous discussion, it can be written as $F_A (1 – X_A)$.

Now on putting the values of moles at the outlet of the reactor in the performance equation and sometimes we need to rearrange the thing. So, this can be written as F_{A0} sorry this is V. So, this is you can say that the better approach for achieving the design equation for a single reaction system.

$$F_{A_o} X_A = -r_A V$$

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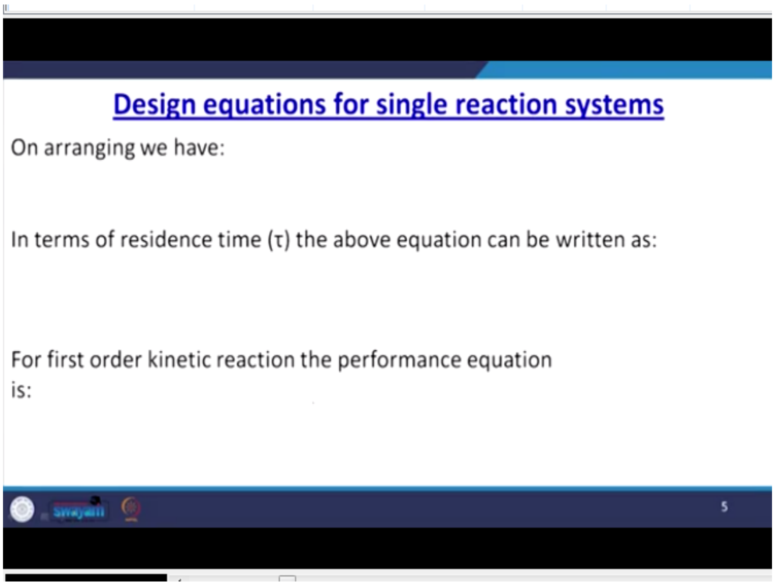

Design equations for single reaction systems

On arranging we have:

In terms of residence time (τ) the above equation can be written as:

For first order kinetic reaction the performance equation is:

Now, if we try to rearrange the things, so, upon rearranging we can write this like F_{A0}. Now, in terms of residence time tau that these equations can be written as tau = V upon mu V upon F_{A0} C_A into V C_{A0} C_{A0} C_{A0} X_A upon - r_A and that is equal to C_{A0} - C_A. So, this is the equation with respect to the residence time. Therefore, based on these particular approaches the first order kinetic reaction or the performance equation can be written as tau = C_{A0} - C_A upon kC_A or k tau = C_{A0} - C_A upon C_A.

On arranging we have

$$\frac{X_A}{-r_A} = \frac{V}{F_{A_o}}$$

If in terms of residence time (τ) the above equation can be written as

$$\tau = \frac{V}{v} = \frac{VC_{A_o}}{F_{A_o}} = \frac{C_{A_o}X_A}{-r_A} = \frac{C_{Ao}\text{-}C_A}{-r_A}$$

For first order kinetic reaction the performance equation is

$$\tau = \frac{C_{Ao}\text{-}C_A}{kC_A}$$

Or

$$\Rightarrow k\tau = \frac{C_{A_o} - C_A}{C_A}$$

So, this is our basic performance equation for the first order kinetic reaction. Now, sometimes we need to draw or we need to put the graphical representation of these performance equations under the head of MFR.

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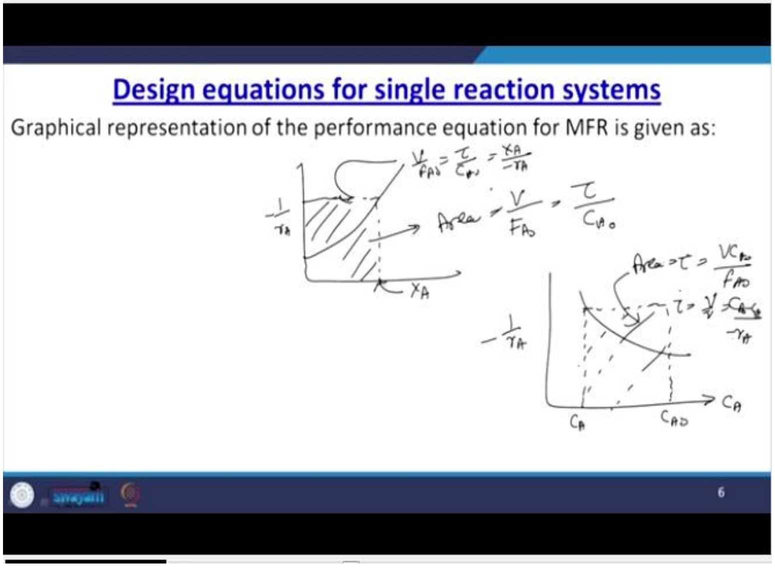

Design equations for single reaction systems

Graphical representation of the performance equation for MFR is given as:

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

$\text{Area} = \frac{V}{F_{A0}} = \frac{\tau}{C_{A0}}$

$\text{Area} = \tau = \frac{V C_{A0}}{F_{A0}}$

$\tau = \frac{V}{v} = \frac{C_{A0} - C_A}{-r_A}$

So, we can easily plot these things with respect to the mole upon and this is the character of this, but these reactions are these equations are like this. Now, here this is X_A and this area under curve is equal to V upon F_{A0} is equal to tau upon C_{A0}.This is represented as V upon F_{A0} tau upon C_{A0} is equal to $X_A/-r_A$. Now, another approach is like this with respect to the concentration. Now, here if you see now, this area tau = V C_{A0} upon F_{A0} or sometimes referred to as tau = V upon v C_{A0} - C_A upon - r_A.

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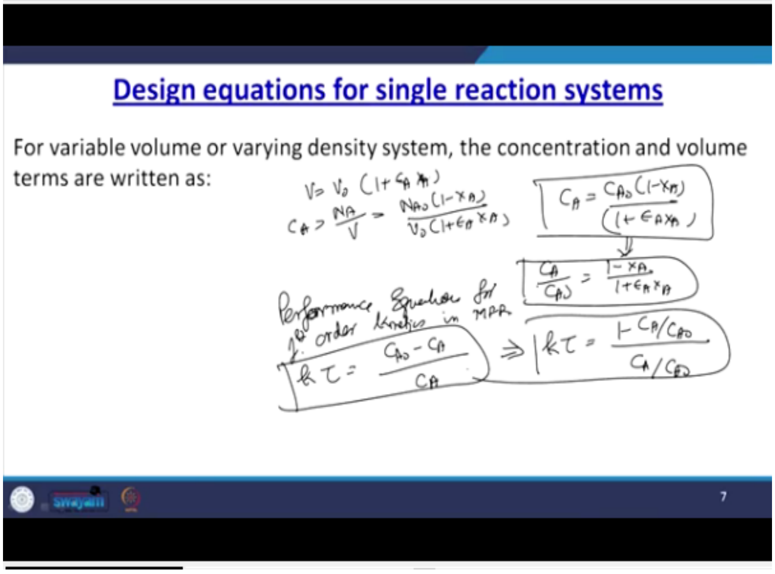

Design equations for single reaction systems

For variable volume or varying density system, the concentration and volume terms are written as:

$V = V_0 (1 + \epsilon_A X_A)$

$C_A = \frac{N_A}{V} = \frac{N_{A0}(1 - X_A)}{V_0(1 + \epsilon_A X_A)}$

$\boxed{C_A = \frac{C_{A0}(1 - X_A)}{(1 + \epsilon_A X_A)}}$

$\Downarrow$

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

Performance Equation for 1st order kinetics in MFR

$\boxed{k\tau = \frac{C_{A0} - C_A}{C_A}} \Rightarrow \boxed{k\tau = \frac{1 - C_A/C_{A0}}{C_A/C_{A0}}}$

So, this is the basic approach for the graphical representation of mixed flow reactor. Now, for the varying volume system or the varying volume or varying density system, the concentration and volume terms you can write like this V = V_0 (1 + epsilon A X_A).

If for variable volume or density system, the concentration and volume terms are written as

$$\frac{\mathrm{V}}{\mathrm{V_o}} = (1 - \mathrm{X_A})$$

The concentration of reactant A can be written as

$$C_A = \frac{N_A}{V} = \frac{N_{A_o}(1 - X_A)}{V_o(1 + \mathcal{E}_A X_A)}$$

$$\frac{C_A}{C_{A_o}} = \frac{(1 - X_A)}{1 + \varepsilon_A X_A}$$

Now, this is represented as N_{A0} (1 - X_A) upon V not (1 + epsilon X_A) or this we can write easily as C_A = C_{A0} (1 - X_A) upon (1 + epsilon A X_A) or sometimes referred as C_A upon C_{A0}(1 - X_A) upon (1 + epsilon A X_A).

So, this is now based on this the performance equation for first order kinetics in MFR, you can write like this k tau C_{A0} or in other words we can put like this 1 - C_A upon C_{A0}. So, these 2 are the performance equation.

Performance equation for first order reaction can be written as

$$\mathrm{k\tau} = \frac{\mathrm{C_{A_o}} - \mathrm{C_A}}{\mathrm{C_A}}$$

Or on simplification we can write it as

$$\mathrm{k\tau} = \frac{1 - \mathrm{C_A}/\mathrm{C_{A_o}}}{\mathrm{C_A}/\mathrm{C_{A_o}}}$$

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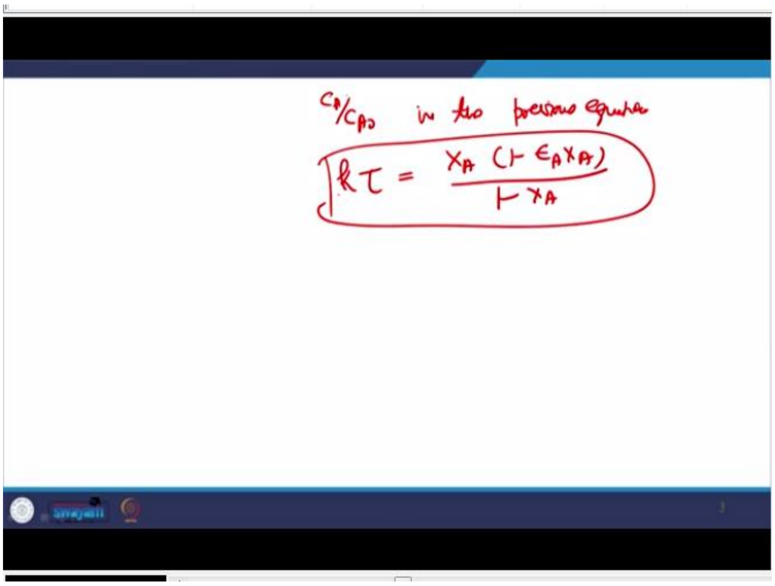

C_A/C_{A0} in the previous equation

$$\boxed{k\tau = \frac{X_A(1+\varepsilon_A X_A)}{1-X_A}}$$

Now, put the values of C_A upon C_{A0} in the previous equation. So, if we put all these values and if you go on the rearranging the aspect then it can be written as k X_A upon 1 - X_A. Now, this is the required performance equation for first order and varying volume system in MFR. So, this is I can see a very important equation related to the mix flow reactor.

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

Now, we have discussed the mixed flow reactor. Now, let us have a look about the plug flow reactor in this regard and we will discuss about the various design equation for the PFR.

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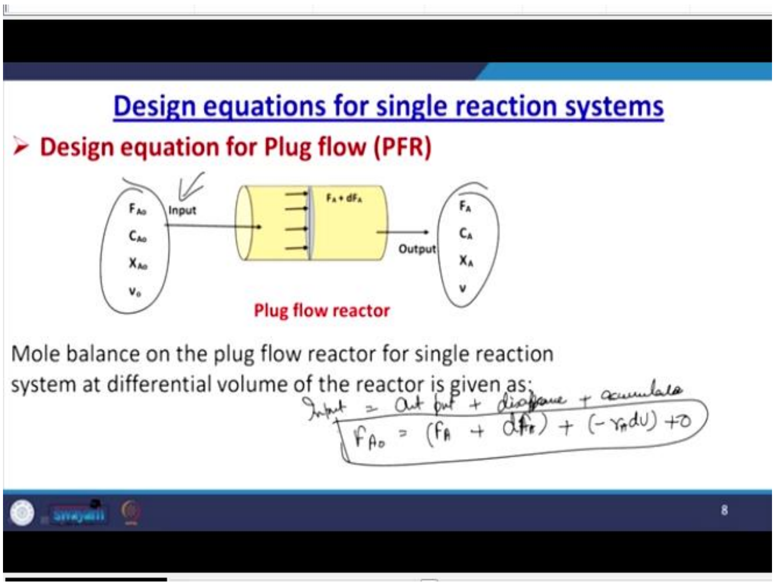

Design equations for single reaction systems

- Design equation for Plug flow (PFR)

Mole balance on the plug flow reactor for single reaction system at differential volume of the reactor is given as:

Input = Out put + disappeance + accumulate

$$\boxed{F_{A_0} = (F_A + dF_A) + (-r_A dV) + 0}$$

Now, this is our general PFR. Now, mole balance if you write the mole balance equation on the plug flow reactor for a single reaction system at various differential level. So, we can easily write that input is equal to output plus disappearance plus accumulation. Now, this can be written as F_{A0} based on this particular approach $F_{A0} = F_A$ + rate of disappearance - r_A dv + 0. So, this is my basic equation or the mole balance equation for this particular approach.

Mole balance on the plug flow reactor for single reaction system at differential volume of the reactor is

Input=output+disappearance+accumulation

$$F_A = F_A + dF_A + (-r_A\ dV) + 0$$

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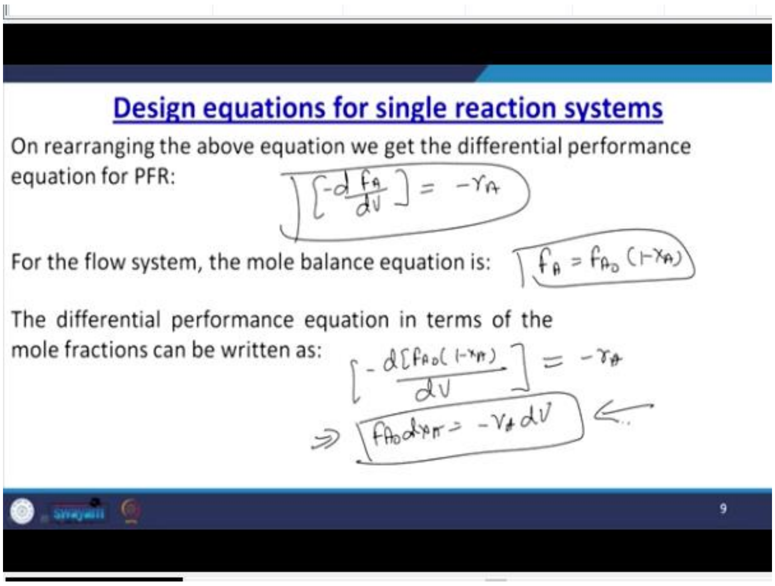

Design equations for single reaction systems

On rearranging the above equation we get the differential performance equation for PFR:

$$\boxed{\left[-\frac{d\,f_A}{dV}\right] = -r_A}$$

For the flow system, the mole balance equation is: $\boxed{f_A = f_{A_0}(1-X_A)}$

The differential performance equation in terms of the mole fractions can be written as:

$$\left[-\frac{d[f_{A0}(1-X_A)]}{dV}\right] = -r_A$$

$$\Rightarrow \boxed{f_{A0}\,dX_A = -r_A\,dV} \leftarrow$$

Now, if we rearrange the given equation, we can get the formal equation based on this particular discussion and this will be - dF_A upon dV. This is based on the rearrangement.

On rearranging the above equation, we get the differential performance equation

$$\left[-\frac{\mathrm{d}\,F_A}{\mathrm{dV}}\right] = -r_A$$

Now, for the flow system the mole balance equation can be represented as $F_A = F_{A0}\,(1 - X_A)$. Now, the performance equation based on the differential form and terms of a mole fraction this can be written like this – $d(F_{A0}\,(1 – X_A))$ upon dV is equal to $-r_A$.

Now, this term is equal to this one. So, therefore, $F_{A0}\,dX_A = -r_AdV$. This is the differential form of the performance equation with respect to the mole fraction.

For the flow system, the mole balance equation is

$$\mathrm{F}_A = F_{A_o}(1 - X_A)$$

From the above two equations, the differential performance equation in terms of the mole fractions can be written as

$$\left[-\frac{\mathrm{d}\,\left(F_{A_o}(1 - X_A)\right)}{\mathrm{dV}}\right] = -r_A$$

$$\mathrm{F}_{A_o}\mathrm{dX}_A = -r_A\mathrm{dV}$$

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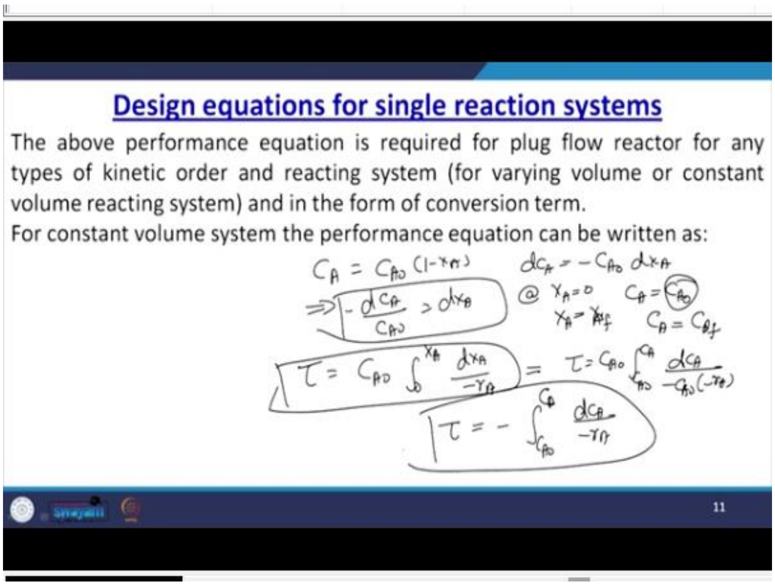

Design equations for single reaction systems

The above performance equation is required for plug flow reactor for any types of kinetic order and reacting system (for varying volume or constant volume reacting system) and in the form of conversion term.

For constant volume system the performance equation can be written as:

$C_A = C_{A0}(1-x_A)$ $\quad dC_A = -C_{A0}\,dx_A$

$\Rightarrow \boxed{-\frac{dC_A}{C_{A0}} = dx_A}$ $\quad$ @ $x_A = 0$ $\quad C_A = \boxed{C_{A0}}$

$x_A = x_{Af}$ $\quad C_A = C_{Af}$

$\boxed{\tau = C_{A0}\int_0^{x_A}\frac{dx_A}{-r_A}} = \tau = C_{A0}\int_{C_{A0}}^{C_A}\frac{dC_A}{-C_{A0}(-r_A)}$

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

And plug flow system the reactants usually are consumed and converted into the product usually as it moves through the reactor length and the final conversion cannot end at the output of that reactor. So, if we try to integrate the things the previous this particular differential equation and for the whole reactor volume so, the final conversion if we are interested in the final conversion X_A.

So, write we can put the things like this F_{A0} dV. Now, this we can write like this dX_A or in front term C_{A0} 0 to X_A dX_A upon - r_A. So, this is my final conversion X_A with respect to the final conversion. Now, let us have a look about the constant volume system. Now, these are performance equation is usually required in a plug flow reactor for any type of kinetic order and the reacting system.

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

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

$$\Rightarrow \tau = C_{A_o}\int_0^{X_A}\frac{dX_A}{-r_A}$$

Now, for varying volume or a constant volume reacting system or it may be in the form of a convergent term. So, if we discuss about the constant volume system under the head of a polymer reactor the performance equation, we can we can write like this $C_A = C_{A0}(1 - X_A)$ or

dC_A - C_{A0} dXC dC_A C_{A0}. Now at X_{A0} is 0 at the start up and then C_A will be equal to C_{A0}, that is the initial concentration of reactant A and in this case, this is the monomer.

As for constant volume system

$$C_A = C_{A_o}(1\text{-}X_A)$$

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

And if we achieve after say time t is X A f or the final concentration of the monomer would be C Af. So, on putting this reaction of the performance relation of the performance equation we may have tau = C_{A0} 0 X_A dX_A - r_A or C_{A0} C_A. This is the final one and dC_A A 0 - r_A So, the performance equation in terms of concentration for constant volume or density system can be written as C_{A0}, that is the initial concentration and then this is the final one and then it is represented like this.

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

So, it is a very useful equation with respect to the predicting the final concentration under the head of plug flow polymerization reaction. Now, if we try to represent with respect to the graphical approach.

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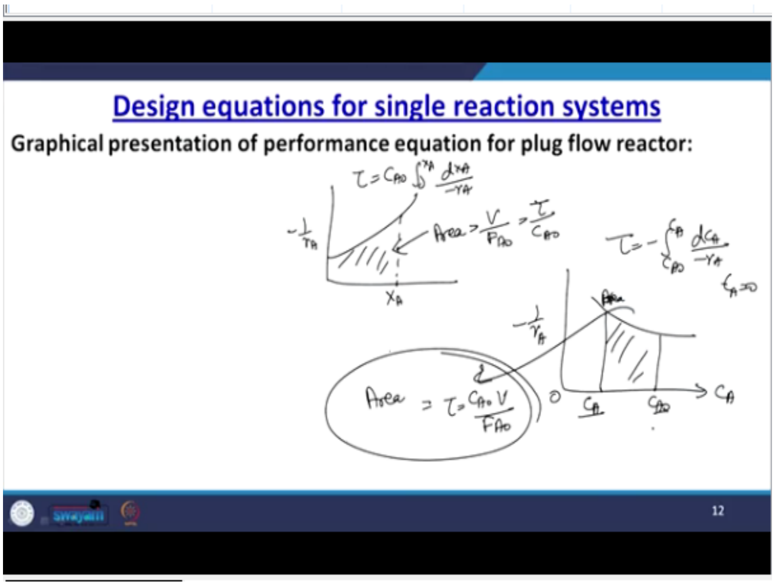

Design equations for single reaction systems

Graphical presentation of performance equation for plug flow reactor:

Then we can put like this and this is the truly experimental approach like this. Now, we are having tau = C_{A0} 0 to X_A dX_A upon - r_A. Now, for any epsilon we can write the area = V upon F_{A0} = tau /C_{A0}. And if we wish to have with respect to the concentration term, then this can be represented with respect to the concentration of monomer A. Then it is like this, this is the initial concentration and over the period of time the concentration of monomer A got depleted.

So, the area then tau equal to minus integration from initial to say final dC_A/r_A. Now, if we have this one, so, area under curve will give you let me put over here, area will give you tau = C_{A0} V upon F_{A0}. So, this is the graphical representation of the performance equation of any kind of a polymerization reaction in the head of plug flow reactor. Now, for variable volume system which we discussed in the previous lecture, you can put the concentration of the variable volume in the rate of performance equation for varying volume. Now, therefore, the performance equation under the head of first order irreversible reaction can be generated under the ages of varying volume. Let us have a look about this one.

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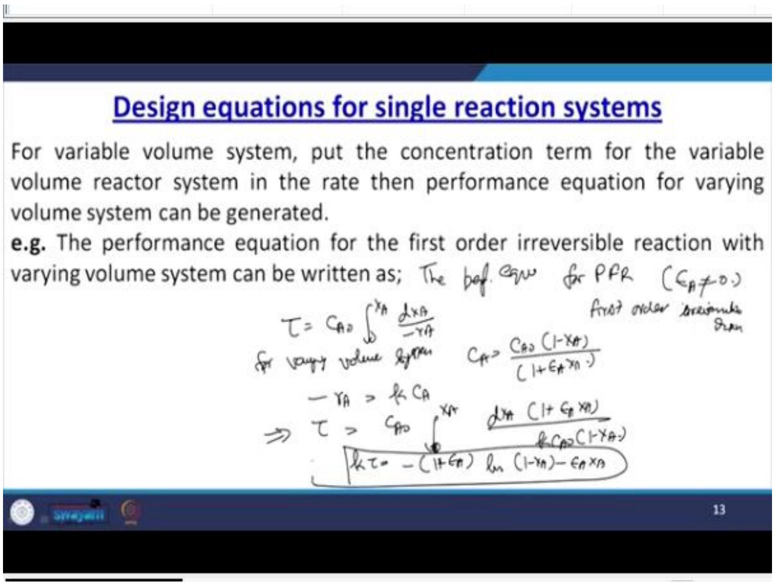

Design equations for single reaction systems

For variable volume system, put the concentration term for the variable volume reactor system in the rate then performance equation for varying volume system can be generated.

e.g. The performance equation for the first order irreversible reaction with varying volume system can be written as; The perf. eqn for PFR ($\epsilon_A \neq 0$) first order irreversible system

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

for varying volume system $C_A = \frac{C_{A0}(1-X_A)}{(1+\epsilon_A X_A)}$

$$-r_A = kC_A$$

$$\Rightarrow \tau = C_{A0}\int_0^{X_A}\frac{dX_A(1+\epsilon_A X_A)}{kC_{A0}(1-X_A)}$$

$$\boxed{k\tau = -(1+\epsilon_A)\ln(1-X_A) - \epsilon_A X_A}$$

Now, the performance equation for PFR where we have this, that is the first order irreversible reaction. So, tau = C_{A0} dX_A Now, for varying volume system C_A = C_{A0} (1 - X_A) upon (1 + epsilon A X_A).

$$\frac{C_A}{C_{A_0}} = \frac{(1 - X_A)}{1 + \varepsilon_A X_A}$$

Now, according to the rate law we can write - r_A = kC_A or tau = C_{A0} integration because initially the moles of A was 0 then X_A then dX_A 1 + epsilon A X_A upon kC_{A0} (1 - X_A).

$$\Rightarrow \tau = C_{A_0}\int_0^{X_A}\frac{\mathrm{d}X_A(1 + \varepsilon_A X_A)}{kC_{A_0}(1 - X_A)}$$

So, if we solve this and rearrange the thing accordingly, so, the final equation will come out to be k tau = 1 + epsilon A ln 1 - X_A - epsilon A X_A. So, this is my required performance equation for the first order with the varying volume system. So, this is according to this, this varying volume and we are considering the plug flow reactor, it is very useful equation especially when we carry out any kind of a polymerization reaction within the thing. Now, come to the last segment of this particular lecture that is that this equation for semi batch reactor.

$$k\tau = -(1+\varepsilon_A)\ln(1-X_A) - \varepsilon_A X_A$$

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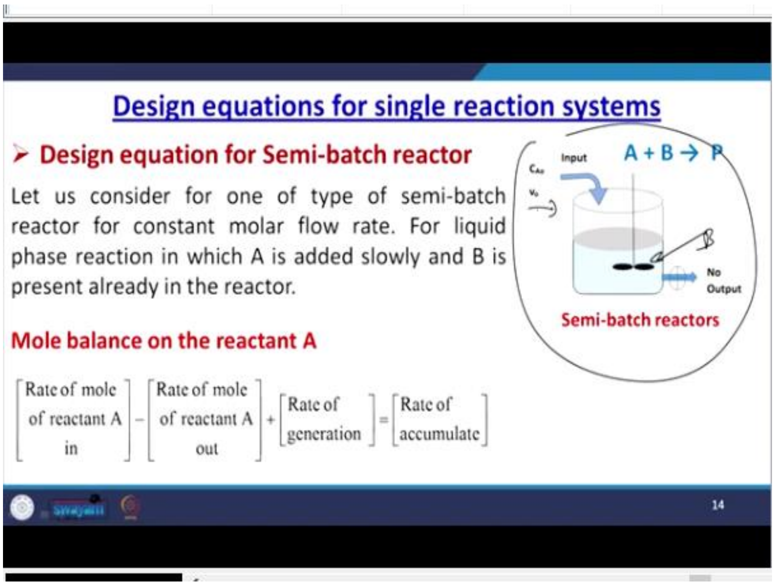

Design equations for single reaction systems

- **Design equation for Semi-batch reactor**

Let us consider for one of type of semi-batch reactor for constant molar flow rate. For liquid phase reaction in which A is added slowly and B is present already in the reactor.

Mole balance on the reactant A

$$\begin{bmatrix}\text{Rate of mole}\\ \text{of reactant A}\\ \text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate of mole}\\ \text{of reactant A}\\ \text{out}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{generation}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{accumulate}\end{bmatrix}$$

We have already gone through the concept of the semi batch reactor. Now, let us consider one of any type of semi batch data for the constant molar flow rate, for liquid phase reaction in which A is continuously added to the slowly and B is already present in this reaction. So, the generalized mole balance on the reactant can be written as the rate of mole of reactant A, whatever going inside minus rate of moles of reactants.

Those were out plus rate of generation equal to the rate of accumulation. So, this is a very broad thing, now, if we try to write the mole balance based on the reactant A, which was added slowly with the molar flow rate of F_{A0}.

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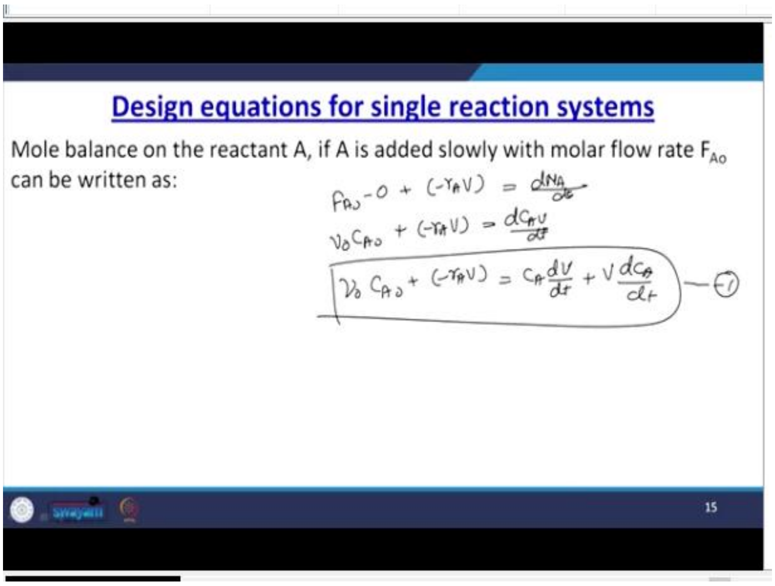

Design equations for single reaction systems

Mole balance on the reactant A, if A is added slowly with molar flow rate F_{Ao} can be written as:

$$F_{Ao} - 0 + (-r_A V) = \frac{dN_A}{dt}$$

$$v_0 C_{Ao} + (-r_A V) = \frac{dC_A V}{dt}$$

$$\boxed{v_0 C_{Ao} + (-r_A V) = C_A \frac{dV}{dt} + V \frac{dC_A}{dt}} \quad \text{--- ①}$$

This can be written as FA0 - 0 + -rAV = dNA and dt. So, with respect to the concentration we can write like this. So, if you differentiate the above equation and try to rearrange the things, we may have this final equation CA V dV dt plus this one d CA dt. So, let us put this equation as equation number 1.

Mole balance on the reactant A

$$\begin{bmatrix}\text{Rate of mole}\\ \text{of reactant A}\\ \text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate of mole}\\ \text{of reactant A}\\ \text{out}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{generation}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{accumulate}\end{bmatrix}$$

$$[F_{\mathrm{Ao}}] - [0] + [(\text{-}r_A V)\ ] = \left[\frac{\mathrm{dN}_A}{\mathrm{dt}}\right]$$

$$\Rightarrow v_o C_{A_o} + (-r_A V) = \frac{d(C_A V)}{\mathrm{dt}}$$

on differentiating and rearranging it, we have

$$\Rightarrow v_o C_{A_o} + (-r_A V) = C_A \frac{d(V)}{\mathrm{dt}} + V \frac{d(C_A)}{\mathrm{dt}}$$

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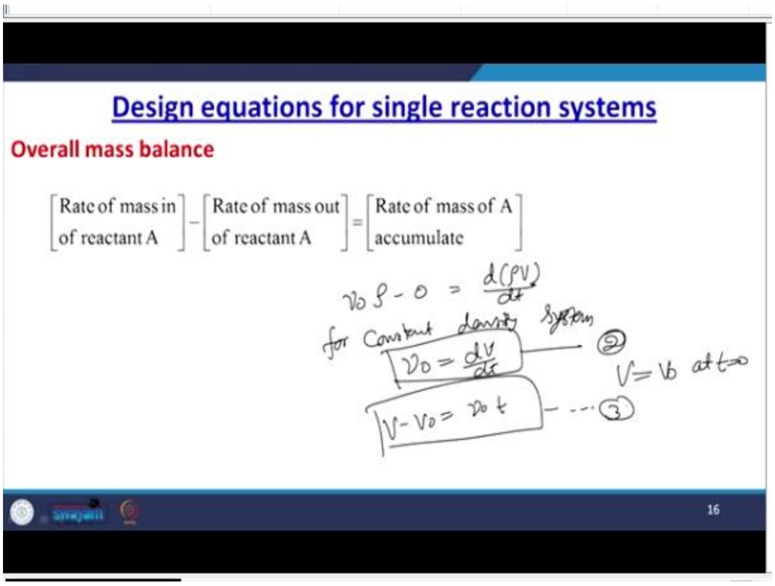

Design equations for single reaction systems

Overall mass balance

$$\begin{bmatrix}\text{Rate of mass in}\\ \text{of reactant A}\end{bmatrix} - \begin{bmatrix}\text{Rate of mass out}\\ \text{of reactant A}\end{bmatrix} = \begin{bmatrix}\text{Rate of mass of A}\\ \text{accumulate}\end{bmatrix}$$

$$\nu_0 \rho - 0 = \frac{d(\rho V)}{dt}$$

for Constant density System

$$\boxed{\nu_0 = \frac{dV}{dt}} \text{ — } ②$$

$V = V_0$ at $t=0$

$$\boxed{V - V_0 = \nu_0 t} \text{ - - - } ③$$

Now, if we try to write the overall mass balance, then we can write like this was the density. So, for the constant density system this can be represented as like this. Now, if we differentiate with initial concentration say at the start that V was V_0 and at time t = 0. So, we may have V - V_0 is equal to this one, let us put forward as equation number 3.

Overall mass balance

$$\begin{bmatrix}\text{Rate of mass in}\\ \text{of reactant A}\end{bmatrix} - \begin{bmatrix}\text{Rate of mass out}\\ \text{of reactant A}\end{bmatrix} = \begin{bmatrix}\text{Rate of mass of A}\\ \text{accumulate}\end{bmatrix}$$

$$\Rightarrow \nu_o \rho - 0 = \frac{d(\rho V)}{dt}$$

For constant density system

$$\nu_o = \frac{dV}{dt} \qquad (2)$$

Let the density of the reaction mixture be constant then the above equation can be rearranging and integrate with initial condition $V=V_o$ at t=0, we have

$$V - V_o = \nu_o t \qquad (3)$$

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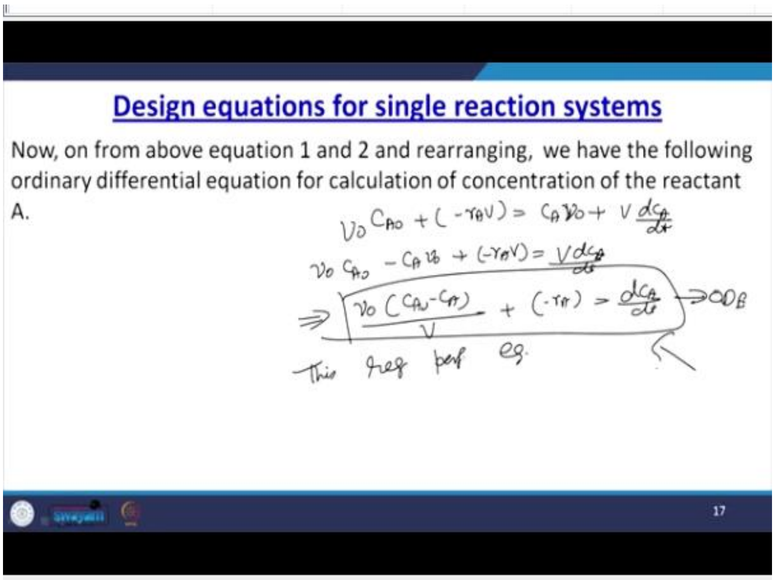

Design equations for single reaction systems

Now, on from above equation 1 and 2 and rearranging, we have the following ordinary differential equation for calculation of concentration of the reactant A.

$$v_0 C_{A0} + (-r_A V) = C_A v_0 + V \frac{dC_A}{dt}$$

$$v_0 C_{A0} - C_A v_0 + (-r_A V) = \frac{V\, dC_A}{dt}$$

$$\Rightarrow \boxed{\frac{v_0 (C_{A0} - C_A)}{V} + (-r_A) = \frac{dC_A}{dt}} \Rightarrow \text{ODE}$$

This req perf eq.

So, if we take the equation number 1 and 2 into cognizance, then we may have you know this C_{A0} + $r_A V$ = C_{A0} + V d C_A dt and nu 0 C_{A0} - C_A nu 0 + V dC_A dt or in other words we may write C_{A0} - C_A V +. So, this is our ordinary differential equation. Now, this is the required performance equation and for the determination of reactant A on concentration pattern. So, this is again a very useful equation related to the reaction engineering especially when we try to design specific polymer reactors.

Now from equation 2 and 1 we have

$$\Rightarrow v_o C_{A_o} - C_A v_o + (-r_A V) = V \frac{d(C_A)}{\mathrm{dt}}$$

$$\Rightarrow \frac{v_o (C_{A_o} - C_A)}{V} + (-r_A) = \frac{d(C_A)}{\mathrm{dt}} \qquad (4)$$

$$\Rightarrow \frac{C_{A_o}}{t} - \frac{C_A}{t} + (-r_A) = \frac{d(C_A)}{\mathrm{dt}} \qquad (5)$$

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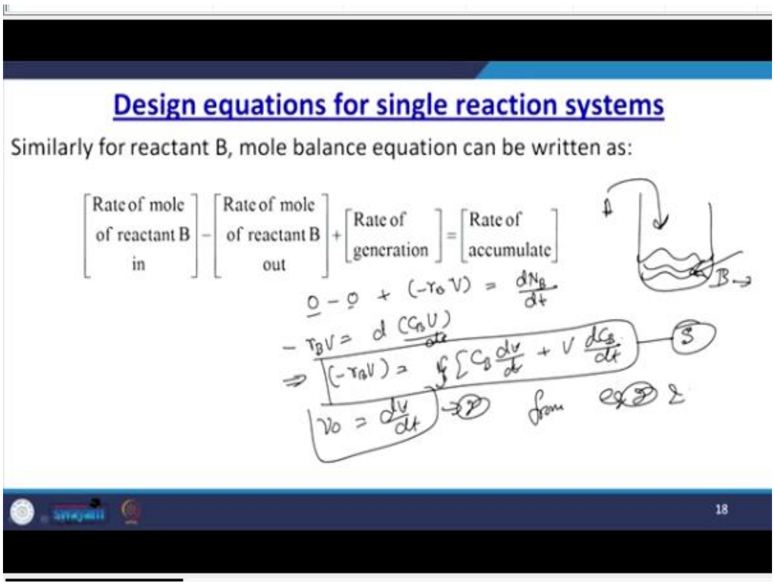

Design equations for single reaction systems

Similarly for reactant B, mole balance equation can be written as:

$$\begin{bmatrix}\text{Rate of mole}\\ \text{of reactant B}\\ \text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate of mole}\\ \text{of reactant B}\\ \text{out}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{generation}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{accumulate}\end{bmatrix}$$

$$0 - 0 + (-r_B V) = \frac{dN_B}{dt}$$

$$-r_B V = \frac{d(C_B V)}{dt}$$

$$\Rightarrow \boxed{(-r_B V) = \left\{C_B \frac{dV}{dt} + V \frac{dC_B}{dt}\right\}} \text{ — } ⑤$$

$$\boxed{v_0 = \frac{dV}{dt}} \rightarrow ②$$

from eq ② &

Now similarly for reactant B; because if you recall that one reactant was within the reactor and other was slowly added to that particular reactor, so, this was your A and this is the B. So, for the other reactant the mole balance equation you can easily write and that is your generic mole balance equation that is a rate of mole of reactant be in and whatever it is coming out plus the rate of generation is equal to rate of accumulation.

So, if we try to find out the mole balance equation around B, then it can be put like this because initially there was no then - r_B V because it is being consumed over the period of time is equal to total number of moles divided by time, then dt. Now this can be put forward like this sorry + V, let us mark this equation as equation number 5. Now, if we recall that we discussed about the equation number 2 over here. So, from equation number we have this dV by dt. So, from equation 2 and 5.

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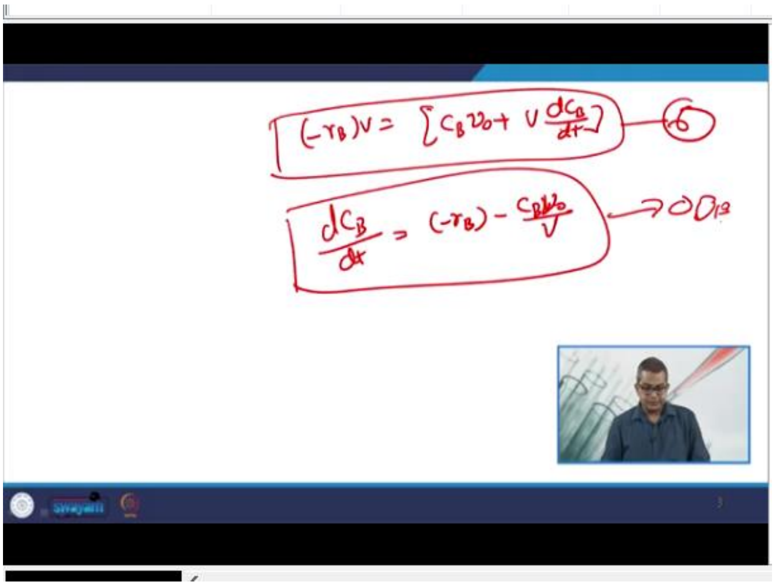

$$\boxed{(-r_B)V = \left[C_B v_0 + V\frac{dC_B}{dt}\right]} \rightarrow ⑥$$

$$\boxed{\frac{dC_B}{dt} = (-r_B) - \frac{C_B v_0}{V}} \rightarrow ODE$$

And if we rearrange the things then we have this - r_B V + V dC_B upon dt. Now, this is my equation number 6. So, if we rearrange the things, then we may have the final equation like V 0 and V. Now, this is the ordinary differential equation and can be solved for the concentration with respect to time.

Similarly for reactant B

$$\begin{bmatrix}\text{Rate of mole}\\ \text{of reactant B}\\ \text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate of mole}\\ \text{of reactant B}\\ \text{out}\end{bmatrix} + \begin{bmatrix}\text{Rate of}\\ \text{generation}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{accumulate}\end{bmatrix}$$

$$[0] - [0] + [\text{-r}_B\text{V}] = \left[\frac{\text{dN}_B}{\text{dt}}\right]$$

$$\Rightarrow [\text{-r}_B\text{V}] = \left[\frac{d(C_B V)}{\text{dt}}\right]$$

$$\Rightarrow [\text{-r}_B\text{V}] = \left[C_B\frac{\text{dV}}{\text{dt}} + V\frac{\text{dC}_B}{\text{dt}}\right]$$

From equation (1) for constant density system $v_o = \frac{\text{dV}}{\text{dt}}$

$$\Rightarrow [\text{-r}_B\text{V}] = \left[C_B v_o + V\frac{\text{dC}_B}{\text{dt}}\right]$$

On rearranging the above equation, we have

$$\Rightarrow \frac{dC_B}{dt} = (-r_B) - \frac{C_B v_o}{V} \qquad (5)$$

These are first order linear differential equation can be solved for the concentration and time required.

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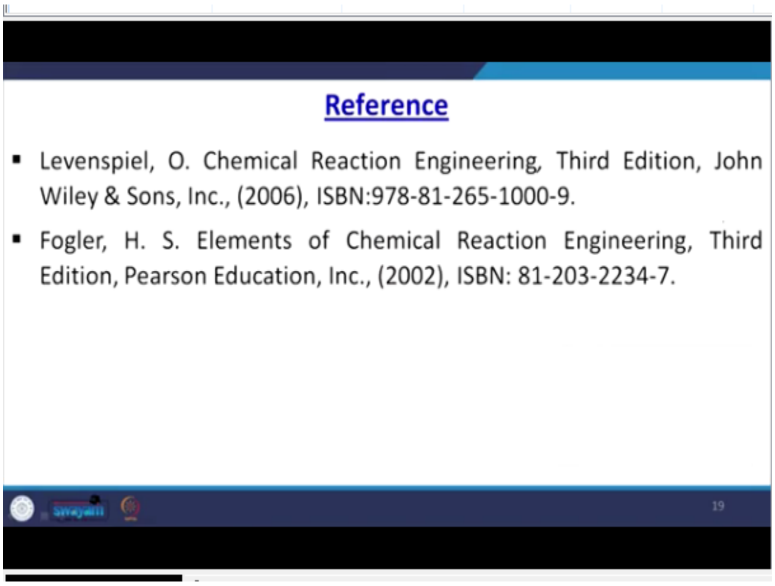

Reference

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- Fogler, H. S. Elements of Chemical Reaction Engineering, Third Edition, Pearson Education, Inc., (2002), ISBN: 81-203-2234-7.

In this particular chapter, we discussed about the various design equation of mixed flow reactor, plug flow reactor, semi batch reactor, which are extremely useful in the various aspect of polymerization process and especially applicable in the industries with respect to the various product profiling. And if you wish to have more and more study in this aspect, we have enlisted several references for your convenience you may go through, thank you very much.