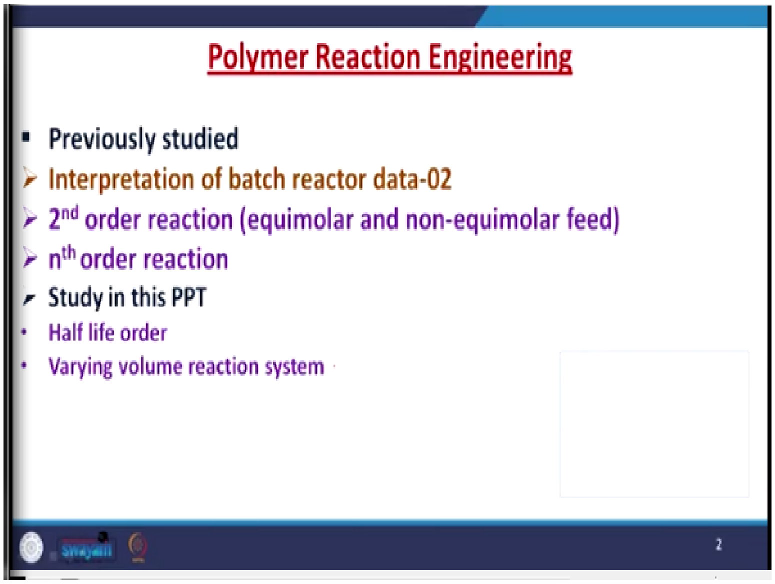
Polymer Reaction Engineering

Prof. Shishir Sinha
Department of Chemical Engineering
Indian Institute of Technology-Roorkee

Lecture-17
Interpretation of Batch Reactor Data-IV

Welcome to the next phase of the interpretation of batch reactor data for reactor design. Now if you recall that previously we have studied about the interpretation pattern of batch reactor data.

(Refer Slide Time: 00:35)



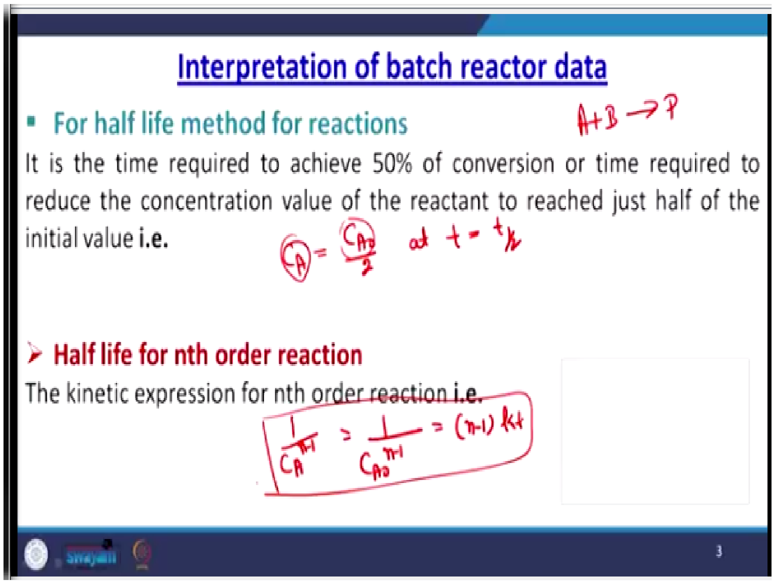
Polymer Reaction Engineering

- Previously studied
- Interpretation of batch reactor data-02
- 2nd order reaction (equimolar and non-equimolar feed)
- nth order reaction
- Study in this PPT
- Half life order
- Varying volume reaction system

Under this head we discussed about the second order reaction, both for equimolar and non-equimolar feed. We developed the mathematical equation for nth order reaction for the prediction of batch reactor data. Now in this particular lecture we will discuss about the half-life order and varying volume reaction system. Both the things are very much important in relation with the batch reactor data and designing of polymer reaction reactors with respect to the product profiling.

Now for half-life method for reactions, now it is as the basic line suggests that it is the time required to achieve 50% of conversion or time required to reduce the concentration value of the reactant to reach just half the initial value. So, if we take the example of our previous reaction that is A + B = P.

(Refer Slide Time: 01:35)



Interpretation of batch reactor data

- For half life method for reactions

$A + B \rightarrow P$

It is the time required to achieve 50% of conversion or time required to reduce the concentration value of the reactant to reached just half of the initial value **i.e.**

$C_A = \frac{C_{A0}}{2}$ at $t = t_{1/2}$

➢ **Half life for nth order reaction**

The kinetic expression for nth order reaction **i.e.**

$\boxed{\frac{1}{C_A^{n-1}} - \frac{1}{C_{A0}^{n-1}} = (n-1)kt}$

Now if we talk about the half-life pattern or half-life method then it may become C_A concentration of reactant A = C_{A0} by 2.

The rate equation for n^th order reaction is written as:

$$-r_A = -\frac{dC_A}{dt} = kC^n{}_A$$

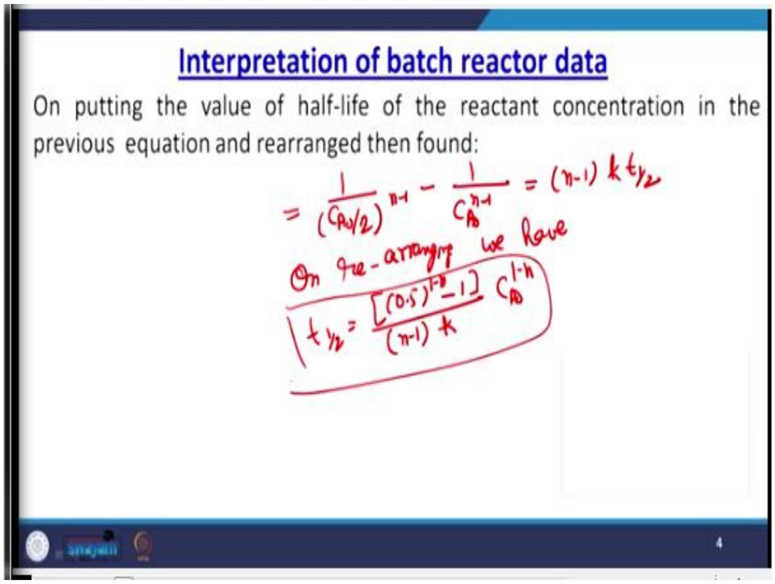
So, at we can say the time t = t, this one, so this is the initial concentration and this is the concentration after t half. So, the kinetic expression for n^th order reaction will become 1 upon C_A^{n-1} -1 upon C_{A0}^{n-1} = (n-1)kt.

$$\frac{1}{C^{n-1}{}_A} - \frac{1}{C^{n-1}{}_{A_0}} = (n-1)kt$$

This equation is valid for $n \neq 1$

So, this equation is representing the n^th order reaction this is the kinetic expression for this half-life prediction.

(Refer Slide Time: 02:34)



Interpretation of batch reactor data

On putting the value of half-life of the reactant concentration in the previous equation and rearranged then found:

$$= \frac{1}{(C_{A0}/2)^{n-1}} - \frac{1}{C_{A0}^{n-1}} = (n-1)\,k\,t_{1/2}$$

On re-arranging we have

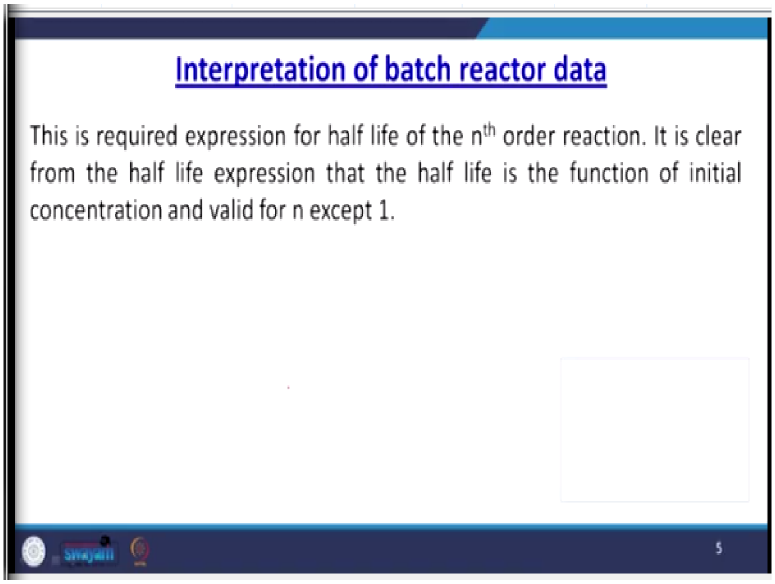
$$\boxed{t_{1/2} = \frac{[(0.5)^{1-n} - 1]}{(n-1)\,k} C_{A0}^{1-n}}$$

Now on putting the value of half-life of the reactant concentration in this equation and try to rearrange, then we found that this equation becomes 1 upon C_{A0} by 2 to the power n - 1 upon C_{A0} n - 1 = n - k t half. So, if we go for the rearrangement 0.5 1 - n - 1 upon n - 1 k C_{A0} 1 - n. So, this is I can say my general equation for predicting this particular half-life pattern of this data.

$$\Rightarrow \quad \frac{1}{\left(C_{A_o}/2\right)^{n\text{-}1}} - \frac{1}{C^{n\text{-}1}{}_{A_o}} = (n-1)kt_{1/2}$$

$$\Rightarrow \quad t_{1/2} = \frac{[(0.5)^{1\text{-}n}\text{-}1]}{(n-1)k} C^{1\text{-}n}{}_{A_o}$$

(Refer Slide Time: 03:42)

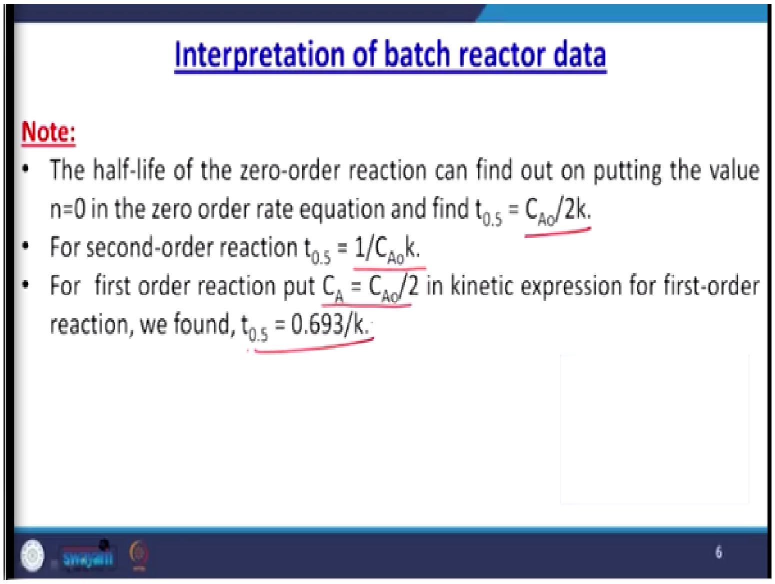


Interpretation of batch reactor data

This is required expression for half life of the n^th^ order reaction. It is clear from the half life expression that the half life is the function of initial concentration and valid for n except 1.

Now this required expression for half-life of nth order reaction, now it is from the half-life expression that the half-life is the function of initial concentration and valid for all kind of n except n is equal to 1. If you see that if you put n = 1, then the entire equation will spoil. So, the half-life of zero order reaction can find out on putting the values of say n = 0 in zero order rate equation and to find out the value of t half at C_{A0} upon 2k.

(Refer Slide Time: 04:23)



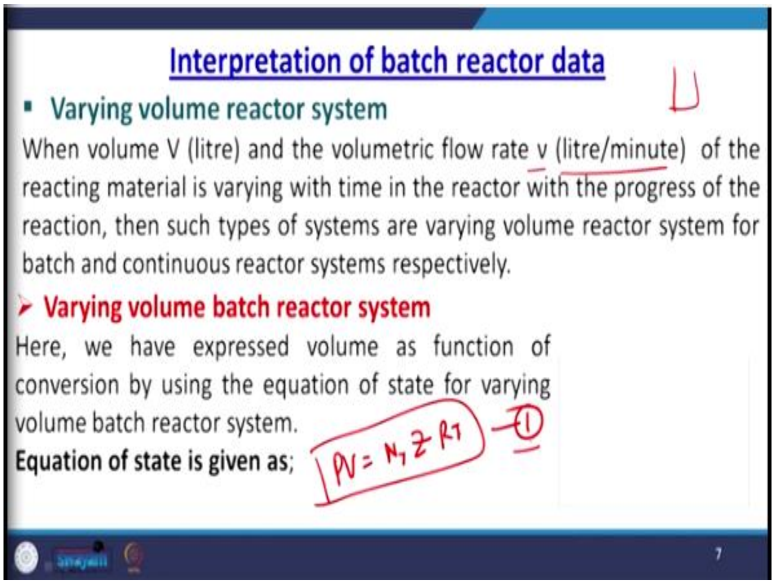
Interpretation of batch reactor data

Note:

- The half-life of the zero-order reaction can find out on putting the value n=0 in the zero order rate equation and find $t_{0.5} = C_{A0}/2k$.
- For second-order reaction $t_{0.5} = 1/C_{A0}k$.
- For first order reaction put $C_A = C_{A0}/2$ in kinetic expression for first-order reaction, we found, $t_{0.5} = 0.693/k$.

Similarly for second order reaction if try to find out the t half that will be 1 upon C_{A0} k. And for the first order reaction if we put the values then $C_A = C_{A0}$ upon 2 in kinetic expression for first order reaction. And if you found that t half = 0.693 upon k, this is a very important result. Now let us come to the last phase of this interpretation of batch reactor data, that is the varying volume or reactor system. So, when volume V that is usually expressed in terms of a unit of a liter.

(Refer Slide Time: 05:20)



Interpretation of batch reactor data

v

- Varying volume reactor system

When volume V (litre) and the volumetric flow rate v (litre/minute) of the reacting material is varying with time in the reactor with the progress of the reaction, then such types of systems are varying volume reactor system for batch and continuous reactor systems respectively.

➢ **Varying volume batch reactor system**

Here, we have expressed volume as function of conversion by using the equation of state for varying volume batch reactor system.

Equation of state is given as; $\boxed{PV = N_T Z RT}$ — ①

And the volumetric flow rate, let us say that having this small v liter per minute of the reacting material is varying with the time in a reactor pattern or reactant system with the progress of the reaction. Then such type of a system they are referred as the varying volume reactor type of system. And it is applicable for both batch and the continuous type of reaction mechanism.

So, I hope that this particular thing is understandable that you are carrying out a reaction in this particular any kind of a reactor. And the volumetric flow rate and volume V, they are into the consideration. And during the progress of the reaction the V and both the volumetric flow rate both are varying due course of time. So, we need to find out the various equation associated with this type of approach.

So, let us have this thing to the consideration for the batch reactor type of system. So, we express the volume as a function of convergent in the previous equation by using the equation of a state for varying volume batch reactor system. Now the equation of a state which attracts our focus that is a $PV = N_TZRT$. Here other things are let us put as equation number 1, pressure, volume, N_T is total number of moles, Z is the compressibility factor, R is universal gas constant or sometimes it is referred as a characteristic gas constant and T is the temperature of the system.

Equation of state;

$$PV = N_T ZRT \qquad (1)$$

Where,

P- total pressure (**kPa**)

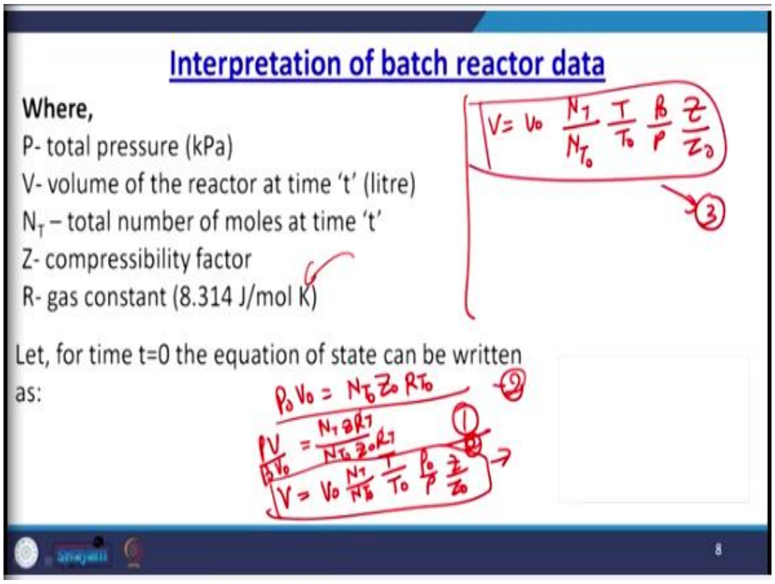
V- volume of the reactor at time ‘t’ (**litre**)

N_T – total number of moles at time ‘t’

Z- compressibility factor

R- gas constant (**8.314 J/mol.K**)

(Refer Slide Time: 06:59)



Interpretation of batch reactor data

Where,

P- total pressure (kPa)

V- volume of the reactor at time ‘t’ (litre)

N_T – total number of moles at time ‘t’

Z- compressibility factor

R- gas constant (8.314 J/mol K)

$$\boxed{V = V_0 \frac{N_T}{N_{T_0}} \frac{T}{T_0} \frac{P_0}{P} \frac{Z}{Z_0}} \rightarrow ③$$

Let, for time t=0 the equation of state can be written as:

$$P_0V_0 = N_{T_0}Z_0RT_0 \quad ②$$

$$\frac{PV}{P_0V_0} = \frac{N_T ZRT}{N_{T_0}Z_0RT} \quad \frac{①}{②}$$

$$\boxed{V = V_0 \frac{N_T}{N_{T_0}} \frac{T}{T_0} \frac{P_0}{P} \frac{Z}{Z_0}} \rightarrow$$

So, this now if see that if we try to find out the situation for time t = 0 the equation of a state we can write as $P_0V_0 = N_{T0}Z_0RT_0$. Remember the P here we are representing P as a total pressure which is represented in equal Pascal, V is the volume of the reactor at time t and already mentioned that it is having the unit of liter. Then N_T is the total number of moles at time t and Z is the compressibility factor and we can put the value of R = 8.314 joule per mole Kelvin.

So, this not represents the initial condition, now if we this is my equation number 2 and if you recall here, we represented the equation number 1. So, if we divide equation 1 by equation 2, then we may have this PV upon P_0V_0 N_T ZRT upon $N_{T0}Z_0$RT. So, if we cancel out these R, so V = V_0 N_T upon N_{T0} this is a subscript T upon T_0P_0 upon P_Z upon Z_0, so this is the generalized equation. To write more clearly it can be represented that V_0NT upon N_{T0} T upon T_0, initial temperature and the final temperature P_0 upon P_Z upon Z_0. Let us refer at this is equation number 3.

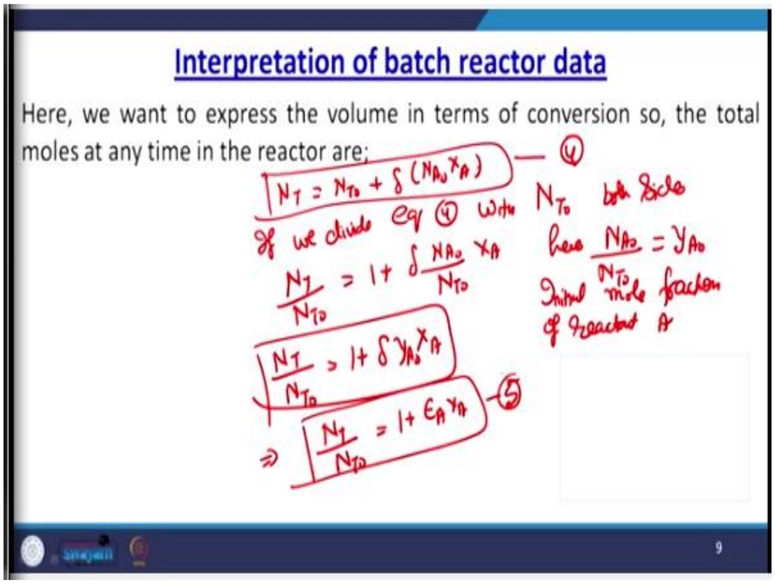
Let for time t=0 the equation of state can be written as:

$$P_o V_o = N_{T_o} \mathrm{ZRT}_o \qquad (2)$$

On dividing previous equation (1) by above equation (2) and rearranging

$$\mathrm{V} = \mathrm{V_o} \frac{\mathrm{N_T}}{\mathrm{N_{T_o}}} \frac{\mathrm{T}}{\mathrm{T_o}} \frac{\mathrm{P}}{\mathrm{P_o}} \frac{\mathrm{Z}}{\mathrm{Z_o}} \qquad (3)$$

(Refer Slide Time: 09:04)



Interpretation of batch reactor data

Here, we want to express the volume in terms of conversion so, the total moles at any time in the reactor are;

$$\boxed{N_T = N_{T_0} + \delta (N_{A_0} X_A)} \text{ — ④}$$

If we divide eq ④ with N_{T_0} both sides

$$\frac{N_T}{N_{T_0}} = 1 + \delta \frac{N_{A_0}}{N_{T_0}} X_A$$

here $\frac{N_{A_0}}{N_{T_0}} = y_{A_0}$ initial mole fraction of reactant A

$$\boxed{\frac{N_T}{N_{T_0}} = 1 + \delta y_{A_0} X_A}$$

$$\Rightarrow \boxed{\frac{N_T}{N_{T_0}} = 1 + \epsilon_A X_A} \text{ — ⑤}$$

Now if we want to express the volume in terms of a conversion, so the total number of moles at any time of the reactor can be given as $N_T = N_{T0}$ change in the number of moles $N_{A0}X_A$, let us put as equation number 4.

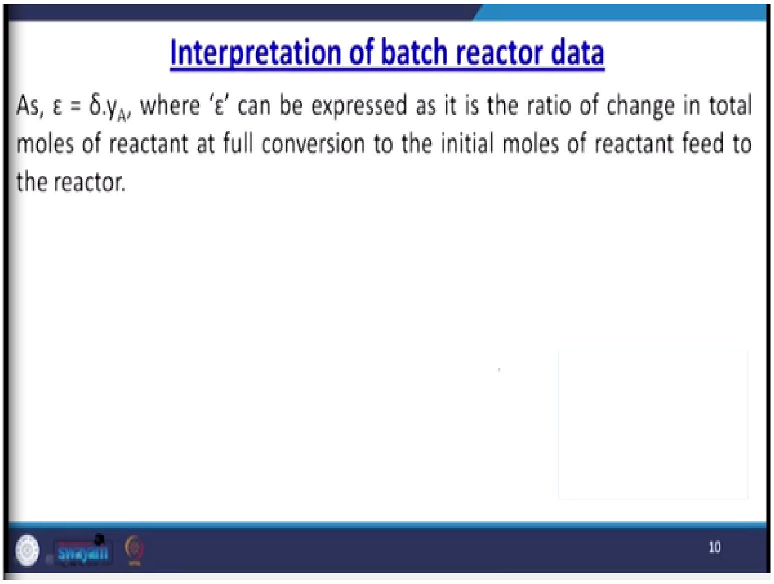
$$\mathrm{N}_T = N_{\mathrm{To}} + \delta (N_{\mathrm{Ao}} X_A) \qquad (4)$$

So, if we divide this equation 4 with N_{T0} to both sides, then N_T upon N_{T0} 1 N_{T0}XA. Now here if you see that N_{A0} upon N_{T0} is Y_{A0}, that is the initial mole fraction, not the mole, initial mole fraction of reactant A.

$$\Rightarrow \quad \frac{N_T}{N_{\mathrm{To}}} = 1 + \delta . \frac{N_{\mathrm{Ao}}}{N_{\mathrm{To}}} X_A \quad (5)$$

Now N_T upon N_{T0} thus become 1 plus change in this pattern X_A or in other words you can see that N_T upon N_{T0} = 1 + epsilon A X_A. Let us represent this particular equation as equation number 5.

(Refer Slide Time: 10:54)



Interpretation of batch reactor data

As, ε = δ.y_A, where 'ε' can be expressed as it is the ratio of change in total moles of reactant at full conversion to the initial moles of reactant feed to the reactor.

Now here if you see that we use the term epsilon, now this epsilon is this delta Y_A, where epsilon can be expressed as the ratio of change in total moles of reactant at full conversion to the initial moles of reactant feed to the reactor. So, this is again we can say it is a very crucial thing and it is very useful for determining the efficacy of any particular reaction.

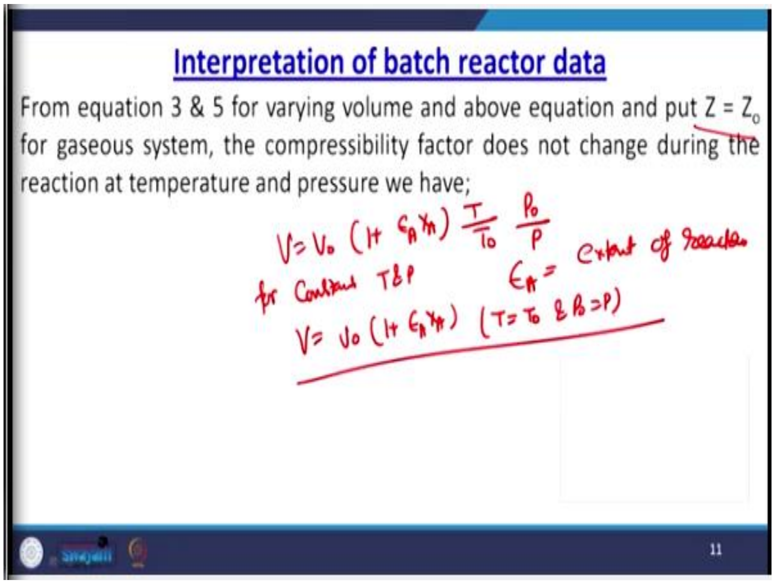
$N_{Ao}/N_{To} = y_{Ao}$ initial mole fraction of reactant A

$$\Rightarrow \quad \frac{N_T}{N_{To}} = 1 + \delta.y_A X_A \quad (6)$$

As, $\varepsilon_A = \delta.y_A$

$$\Rightarrow \quad \frac{N_T}{N_{To}} = 1 + \varepsilon_A X_A$$

(Refer Slide Time: 11:26)



Interpretation of batch reactor data

From equation 3 & 5 for varying volume and above equation and put $Z = Z_0$ for gaseous system, the compressibility factor does not change during the reaction at temperature and pressure we have;

$$V = V_0 (1 + \varepsilon_A X_A) \frac{T}{T_0} \frac{P_0}{P}$$

for Constant T&P

ε_A = extent of reaction

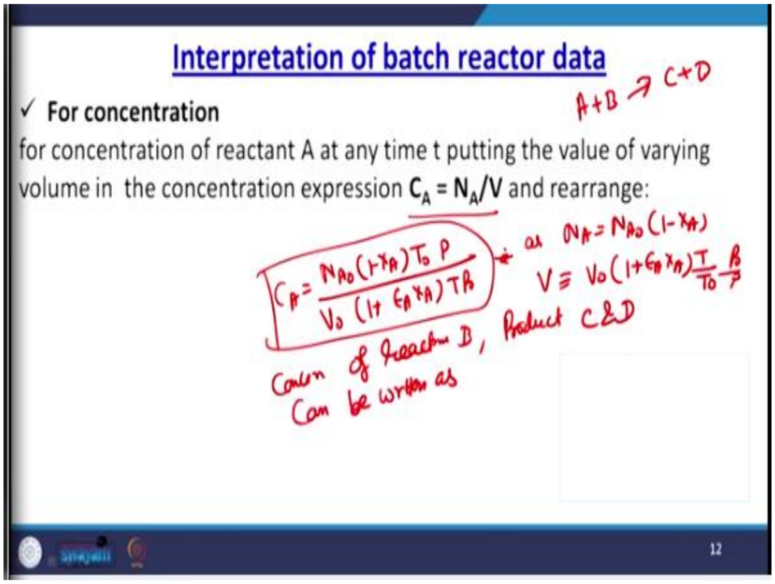
$$V = V_0 (1 + \varepsilon_A X_A) \quad (T = T_0 \;\&\; P_0 = P)$$

Now if you see that from earlier equation number 3, let us go back this is the equation number 3 and equation number 5 which we discussed over here. So, if you see that equation number 3 and 5 for varying volume the above these equations. And if you put $Z = Z_0$ for the gaseous system, the compressibility factor does not change during the reaction at the temperature and pressure, so in that case we have $V = V_0$ 1 + epsilon A $X_A T_0 P_0$ upon P.

$$V = V_o(1 + \varepsilon_A X_A)\frac{T}{T_o}\frac{P}{P_o}$$

Now for constant T and P, and if you see that always we are looking for the extent of a reaction, so epsilon A is represented as the extent of reaction, so $V = V_0$ 1 + epsilon A X_A. Now here the $T = T_0$ and $P_0 = P$, so you see that these things are case sensitive. So, we need to take either certain assumptions or we need to assume the case maybe the gaseous segment maybe for some other segments.

(Refer Slide Time: 13:12)



Interpretation of batch reactor data

✓ **For concentration**

$A + B \rightarrow C + D$

for concentration of reactant A at any time t putting the value of varying volume in the concentration expression $\underline{\mathbf{C_A = N_A/V}}$ and rearrange:

$$\boxed{C_A = \frac{N_{A0}(1-X_A)T_0 P}{V_0(1+\epsilon_A X_A)T P_0}}$$

as $N_A = N_{A0}(1-X_A)$

$V = V_0(1+\epsilon_A X_A)\frac{T}{T_0}\frac{P_0}{P}$

Concn of reactant B, Product C&D Can be written as

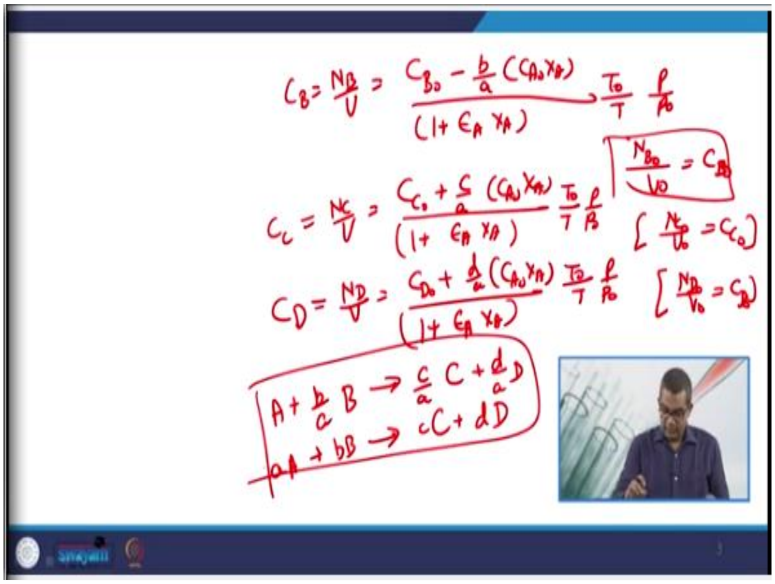
Now as far as the concentration is in question, so for concentration of reactant A at any time you may get the putting the values of varying volume in the concentration expression C_A = N_A upon V. So, this particular equation if you see that C_A can be represented as N_{A0} (1 – X_A) T_0P upon V_0 1 + epsilon A X_A TP_0 plus.

$$C_A = \frac{N_{A_o}(1 - X_A)}{V_o(1 + X_A)} \frac{T_o}{T} \frac{P}{P_o}$$

$$\Rightarrow \qquad C_A = C_{A_o} \frac{(1 - X_A)}{(1 + \varepsilon_A X_A)} \frac{T_o}{T} \frac{P}{P_o}$$

Now this is the general equation or we can represented as N_A = N_{A0} (1 - X_A) or V = V_0 1 + epsilon A X_AT upon T_0P_0 upon P. Now similarly the concentration of reactant B or product C and D if you are having the equation like this.

(Refer Slide Time: 14:27)



$$C_B = \frac{N_B}{V} = \frac{C_{B_0} - \frac{b}{a}(C_{A_0}X_A)}{(1+\epsilon_A X_A)} \frac{T_0}{T} \frac{P}{P_0}$$

$$\boxed{\frac{N_{B_0}}{V_0} = C_{B_0}}$$

$$C_C = \frac{N_C}{V} = \frac{C_{C_0} + \frac{c}{a}(C_{A_0}X_A)}{(1+\epsilon_A X_A)} \frac{T_0}{T} \frac{P}{P_0} \quad \left[\frac{N_{C_0}}{V_0} = C_{C_0}\right]$$

$$C_D = \frac{N_D}{V} = \frac{C_{D_0} + \frac{d}{a}(C_{A_0}X_A)}{(1+\epsilon_A X_A)} \frac{T_0}{T} \frac{P}{P_0} \quad \left[\frac{N_{D_0}}{V_0} = C_{D_0}\right]$$

$$\boxed{\begin{array}{l} A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D \\ aA + bB \rightarrow cC + dD \end{array}}$$

This can be written as $C_B = N_B$ upon V that is C_{B0} – b upon a C_{A0} X_A upon (1 + epsilon A X_A)T_0 upon T P upon P_0, here you see that N_{B0} upon $V_0 = C_{B0}$. Similarly, if we try to write the equation for concentration of C, that is N_C upon V this is equal to N_{C0} + c upon a C_{A0} X_A upon 1 + epsilon A X_A) T_0 upon T P upon P_0. Here N_{C0} upon $V_0 = C_{co}$ concentration at zeroth time.

And last if we try to write the C concentration of D, this is represented as the number of moles of D divided by volume, C_{D0} initial number of moles of component d, d upon a, a is the limiting reactant C_{A0} X_A upon 1 + epsilon A X_A T_0/T P upon P_0, needless to mention that N_{D0} upon V_0 = C_{D0}.

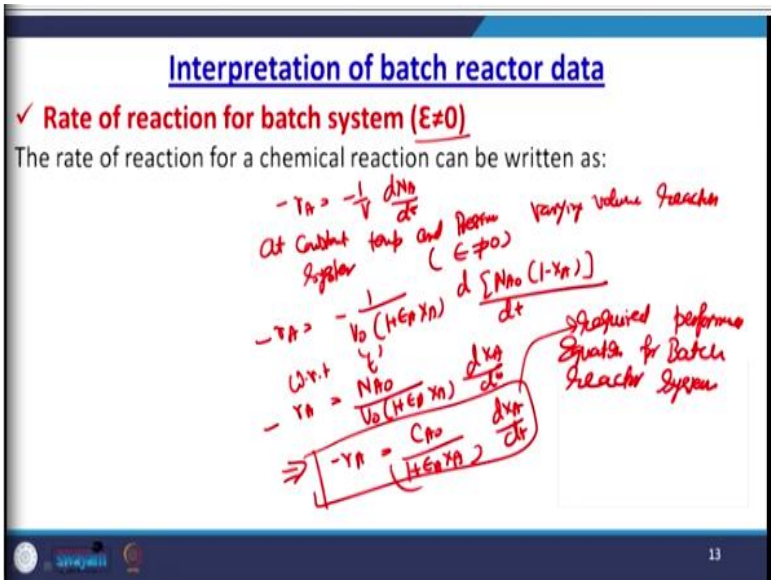
$$C_B = \frac{N_B}{V} = \frac{C_{Bo} - {}^{b}/_{a}\left(C_{A_o}X_A\right)}{(1 + \varepsilon_A X_A)} \frac{T_o}{T} \frac{P}{P_o}$$

$$C_C = \frac{N_C}{V} = \frac{C_{Co} + {}^{c}/_{a}\left(C_{A_o}X_A\right)}{(1 + \varepsilon_A X_A)} \frac{T_o}{T} \frac{P}{P_o}$$

$$C_D = \frac{N_D}{V} = \frac{C_{Do} + {}^{d}/_{a}\left(C_{A_o}X_A\right)}{(1 + \varepsilon_A X_A)} \frac{T_o}{T} \frac{P}{P_o}$$

So, this if you see that we are referring this particular reaction like this b upon a C upon a C + d upon a D, this is based on this particular equation. So, based on this particular approach you can predict the things accordingly. Now if I wish to predict the rate of reaction.

(Refer Slide Time: 16:54)



Interpretation of batch reactor data

✓ Rate of reaction for batch system ($\varepsilon \neq 0$)

The rate of reaction for a chemical reaction can be written as:

$-r_A = -\frac{1}{V}\frac{dN_A}{dt}$

At constant temp and pressure varying volume reaction system ($\epsilon \neq 0$)

$-r_A = -\frac{1}{V_0(1+\epsilon_A X_A)} \frac{d[N_{A0}(1-X_A)]}{dt}$

w.r.t 't'

$-r_A = \frac{N_{A0}}{V_0(1+\epsilon_A X_A)}\frac{dX_A}{dt}$

$\Rightarrow \boxed{-r_A = \frac{C_{A0}}{(1+\epsilon_A X_A)}\frac{dX_A}{dt}}$

Required performance equation for Batch reactor system

13

In that case when usually the epsilon is not equal to 0. So, the rate of a reaction of a chemical reaction you can write as - r_A = -1 upon VdN_A/dt.

$$-r_A = \frac{1}{V}\frac{dN_A}{dt}$$

So, at constant temperature and pressure and for the varying volume system, reaction system where we are considering that is epsilon is not equal to 0. Then - r_A = 1 upon V_0 (1 + epsilon A X_A) d(N_{A0} (1 - X_A) upon dt.

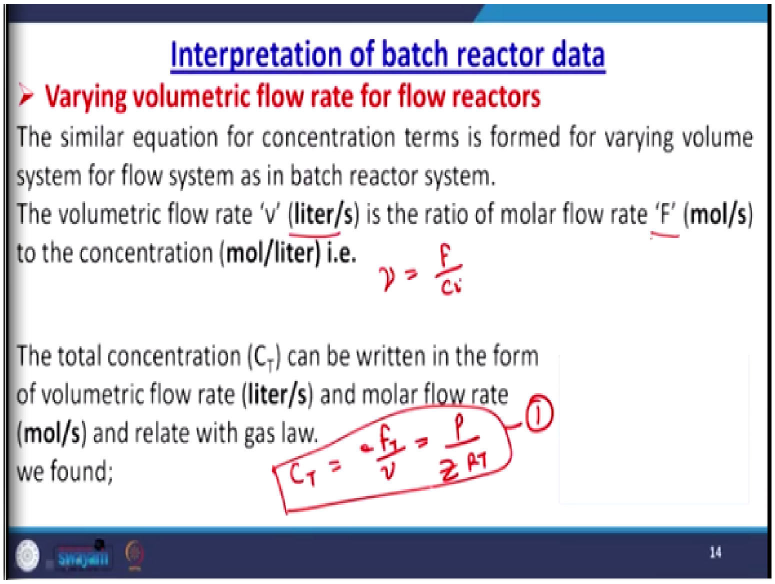
$$-r_A = -\frac{1}{V_o(1+\varepsilon_A X_A)}\frac{d\left(N_{A_o}(1-X_A)\right)}{dt}$$

So, if we differentiate this particular equation with the respect to t, then we may have - r_A and N_{A0} upon V_0 (1 + epsilon A X_A) dX_A upon dt or you can write - r_A = C_{A0} /(1 + epsilon A X_A dX_A upon dt. This is my final equation and this is the required performance equation for batch reactor system.

$$-r_A = \frac{N_{A_o}}{V_o(1+\varepsilon_A X_A)}\frac{dX_A}{dt}$$

$$-r_A = \frac{C_{A_o}}{(1+\varepsilon_A X_A)}\frac{dX_A}{dt}$$

(Refer Slide Time: 18:45)



Interpretation of batch reactor data

- **Varying volumetric flow rate for flow reactors**

The similar equation for concentration terms is formed for varying volume system for flow system as in batch reactor system.

The volumetric flow rate 'v' (**liter/s**) is the ratio of molar flow rate 'F' (**mol/s**) to the concentration (**mol/liter**) **i.e.**

$$\nu = \frac{F}{C_i}$$

The total concentration (C_T) can be written in the form of volumetric flow rate (**liter/s**) and molar flow rate (**mol/s**) and relate with gas law.

we found;

$$\boxed{C_T = \frac{F_T}{\nu} = \frac{P}{ZRT}} \quad ①$$

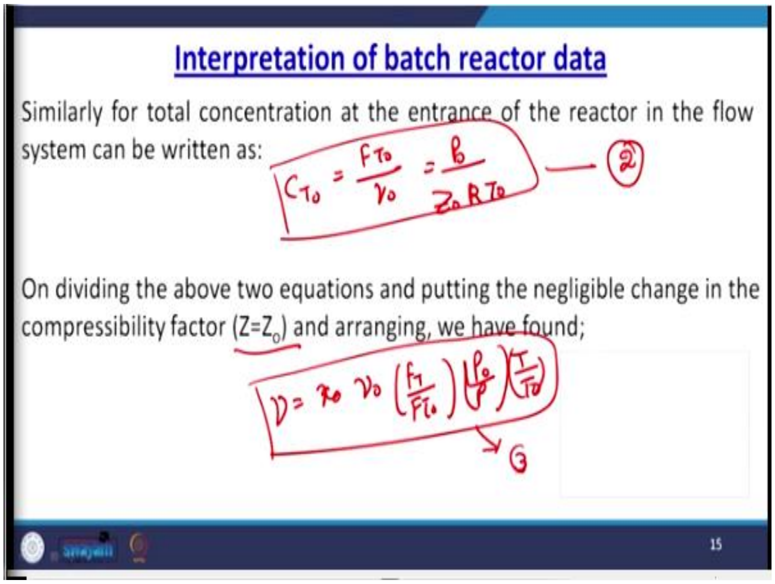
Now again another thing is that if we have the varying volume flow rate for flow reactor. So, this type of similar equation for concentration term is formed for varying volume system, for flow system as in the we observed in the batch reactor system. So, if you have the varying volume in liter per second, this is the ratio of a molar flow rate F that is mole per second to the concentration moles per liter.

$$\text{volumetric flow rate } (\nu) = \frac{F}{C_i}$$

So, sometimes this volumetric flow rate is represented as F upon Ci, i is the i^{th} component. Now if the total concentration of C_T is in question, so the total concentration C_T can be then in the form of a volumetric flow rate and the molar flow rate. And the relate with the gas law, so we can find that total concentration at any time T this is $C_T = F_T$ upon v = P/ZRT, let us put this thing as equation number 1, so this is the total concentration at any time.

$$C_T = \frac{F_T}{\nu} = \frac{P}{ZRT}$$

(Refer Slide Time: 20:07)



Interpretation of batch reactor data

Similarly for total concentration at the entrance of the reactor in the flow system can be written as:

$$\boxed{C_{T_0} = \frac{F_{T_0}}{\nu_0} = \frac{P_0}{Z_0 R T_0}} \longrightarrow ②$$

On dividing the above two equations and putting the negligible change in the compressibility factor ($Z=Z_0$) and arranging, we have found;

$$\boxed{\nu = x_0 \nu_0 \left(\frac{F_T}{F_{T_0}}\right)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)} \rightarrow 3$$

Now, similarly the total concentration at the entrance of the reactor in the flow system, you can write like this because at the entrance of the reactor some of the concentrations maybe put as 0 or not. So, we can write the total concentration at the entrance of the reactor $C_{T0} = F_{T0}$ or P_0 upon Z_0 RT_0.

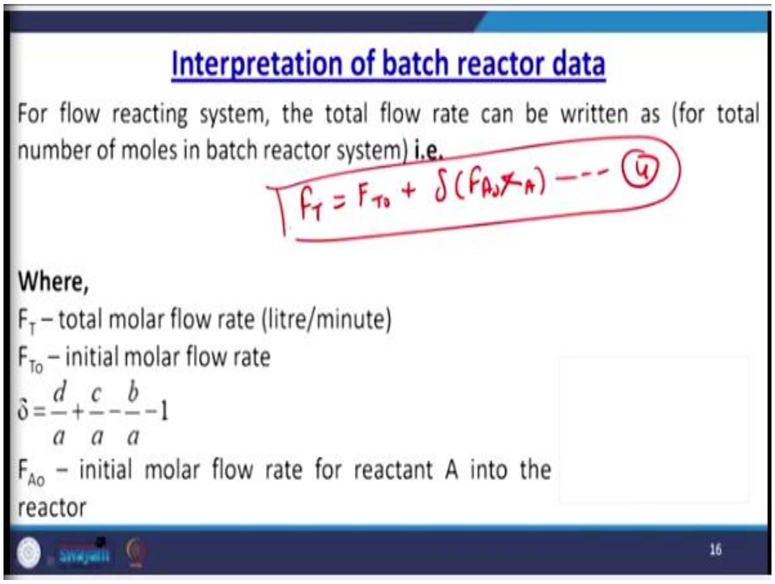
$$C_{T_o} = \frac{F_{T_o}}{\nu_o} = \frac{P_o}{Z_o R T_o}$$

let us refer this particular equation as equation number 2. Now if we divide these two equations and putting the negligible change in the compressibility factor, that is represented as $Z = Z_0$.

And if we try to rearrange and then we find that this is F_T upon F_{T0} P_0 upon P and T upon T_0, so this is my equation and let us put this equation as equation number 3.

$$\nu = \nu_o \left(\frac{F_T}{F_{T_o}}\right)\left(\frac{P_o}{P}\right)\left(\frac{T}{T_o}\right)$$

(Refer Slide Time: 21:19)



Interpretation of batch reactor data

For flow reacting system, the total flow rate can be written as (for total number of moles in batch reactor system) **i.e.**

$$F_T = F_{To} + \delta(F_{Ao}X_A) \text{ --- ④}$$

Where,

F_T – total molar flow rate (litre/minute)

F_{To} – initial molar flow rate

$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$

F_{Ao} – initial molar flow rate for reactant A into the reactor

So, if we talk about the flow reacting system, the total flow rate if we sometimes we may require the total flow rate this can be written as like $F_T = F_{T0} + \delta F_{Ao}X_A$, this is equation number 4.

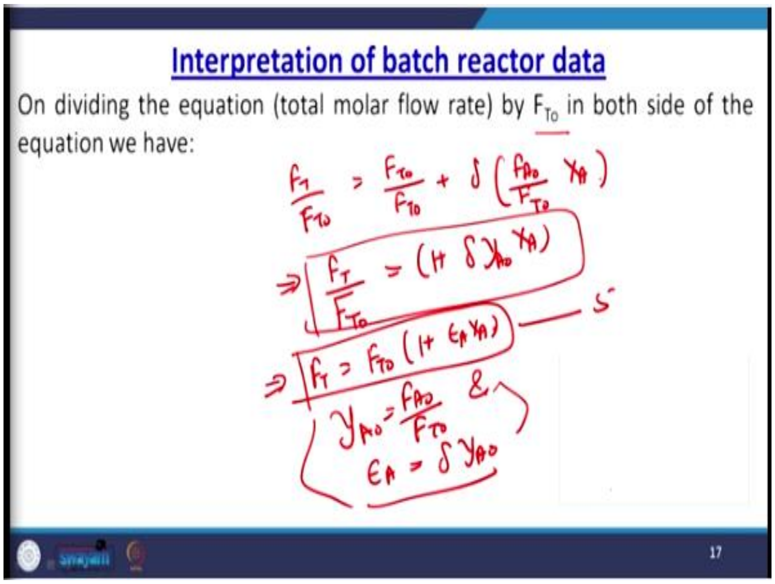
$$F_T = F_{To} + \delta(F_{Ao}X_A)$$

Now here F_T is the total molar flow rate that is represented in liter per minute, then F_{T0} is the initial molar flow rate because we are changing this flow rate or varying flow rate we are considering into question.

Then delta is equal to d upon a + c upon a + - b upon a - 1, now here minus sign is put just to represent that both these reactants are being consuming in due course of time. And F_{A0} is the initial molar flow rate of reactant A into the reactor system.

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

(Refer Slide Time: 22:27)



Interpretation of batch reactor data

On dividing the equation (total molar flow rate) by F_{T_o} in both side of the equation we have:

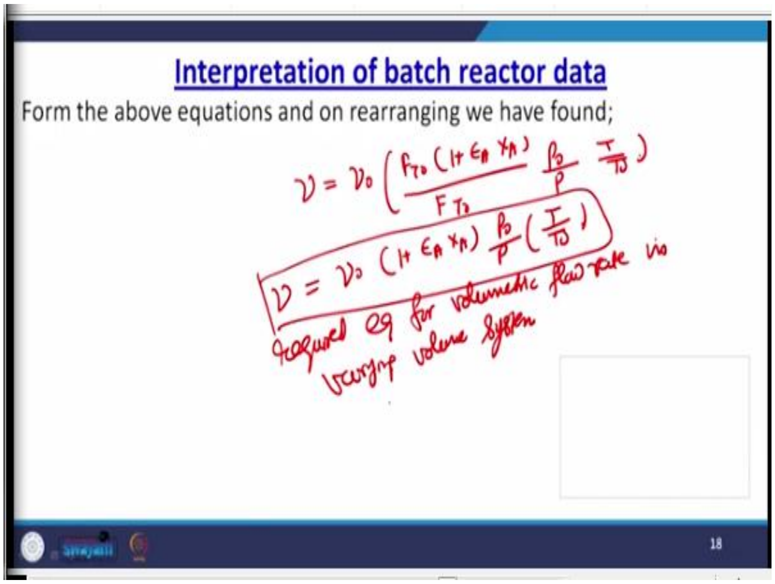
$$\frac{F_T}{F_{T0}} = \frac{F_{T0}}{F_{T0}} + \delta\left(\frac{F_{A0}}{F_{T0}} X_A\right)$$

$$\Rightarrow \boxed{\frac{F_T}{F_{T0}} = (1+\delta y_{A0} X_A)} \text{ — } 5$$

$$\Rightarrow \boxed{F_T = F_{T0}(1+\epsilon_A X_A)}$$

$$y_{A0} = \frac{F_{A0}}{F_{T0}} \ \& \ \epsilon_A = \delta y_{A0}$$

(Refer Slide Time: 22:28)



Interpretation of batch reactor data

Form the above equations and on rearranging we have found;

$$\nu = \nu_0\left(\frac{F_{T0}(1+\epsilon_A X_A)}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0}\right)$$

$$\boxed{\nu = \nu_0 (1+\epsilon_A X_A) \frac{P_0}{P}\left(\frac{T}{T_0}\right)}$$

Required eq for volumetric flow rate in varying volume system

Now we have already from these above equations, now if we divide the equation that is the total molar flow rate by say F_{T0} in both the side of this particular equation. Then the things become like F_T upon F_{T0} = F_{T0} upon + delta F_{A0} upon F_{T0} X_A. And this can be represented like this F_T upon F_{T0} 1 + delta Y mole fraction of A0 into X_A.

On dividing the equation (84) by F_{To} in both side of the equation we have;

$$\frac{F_T}{F_{To}} = 1 + \delta.\frac{F_{Ao}}{F_T} X_A$$

As on putting $y_A = F_{Ao}/F_{To}$ and $\varepsilon = \delta.y_A$ in the above equation we have;

$$F_T = F_{T_0}(1 + \varepsilon X_A)$$

And upon rearranging this $F_T = F_{T0}$ (1 + epsilon A XA), we can put this as equation number 5. So, this here $Y_{A0} = F_{A0}$ upon F_{T0} and epsilon A = delta Y_{A0}, so these are the some of the differencing things.

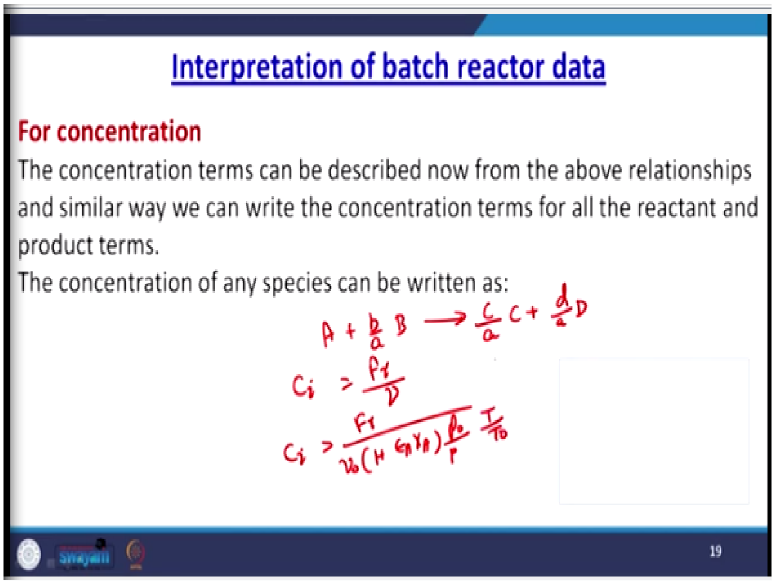
Now from this equation which we discussed and on rearrangement we can have this F_{T0} (1 + epsilon A X_A) upon F_{T0} P_o upon P T upon T_0, so we can represent like this V_0 (1 + epsilon A X_A) P_0 upon P T upon T_0.

$$\nu = \nu_o\left(\frac{F_{T_0}(1 + \varepsilon X_A)}{F_{T_o}}\right)\left(\frac{P_o}{P}\right)\left(\frac{T}{T_o}\right)$$

$$\nu = \nu_o(1 + \varepsilon X_A)\left(\frac{P_o}{P}\right)\left(\frac{T}{T_o}\right)$$

Now this is the required equation for volumetric flow rate in varying volume system. So, this is again a very I can say this is very important relation which we developed in due course of time. Now if we see the concentration effect because we discussed about the varying volume, we discussed about the other factors. Now for the concentration terms can be described now from these relationships which we discussed in the previous slides. And similar way we can write the concentration term for all reactants and other product terms.

(Refer Slide Time: 25:33)



Interpretation of batch reactor data

For concentration

The concentration terms can be described now from the above relationships and similar way we can write the concentration terms for all the reactant and product terms.

The concentration of any species can be written as:

$$A + \frac{b}{a}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D$$

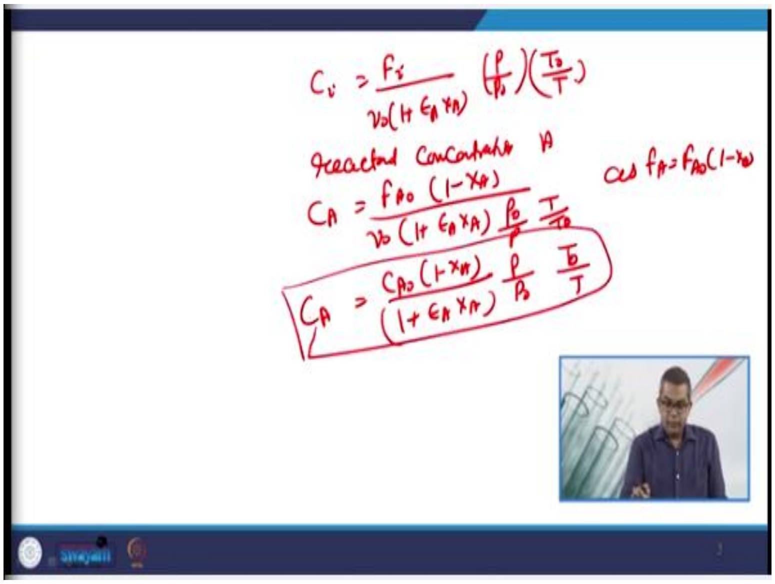
$$C_i = \frac{F_i}{v}$$

$$C_i = \frac{F_i}{v_0(1+\varepsilon_A Y_A)\frac{P_0}{P}\frac{T}{T_0}}$$

So, if we would like to have the concentration of any species which can be written as for this particular equation, we are taking this particular equation into count A + b upon a B c upon a C + d upon D. Now here this is my master equation or sometimes it is referred as Ci Fi upon P_0 into T upon T_0.

$$C_i = \frac{F_i}{\nu} = \frac{F_{io}}{\nu_o(1 + \varepsilon X_A)\left(\frac{P_o}{P}\right)\left(\frac{T}{T_o}\right)}$$

(Refer Slide Time: 26:09)



$$C_i = \frac{F_i}{\nu_0(1+\epsilon_A X_A)}\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)$$

reactant concentration A

$$C_A = \frac{F_{A0}(1-X_A)}{\nu_0(1+\epsilon_A X_A)\frac{P_0}{P}\frac{T}{T_0}}$$

as $F_A = F_{A0}(1-X_A)$

$$\boxed{C_A = \frac{C_{A0}(1-X_A)}{(1+\epsilon_A X_A)}\frac{P}{P_0}\frac{T_0}{T}}$$

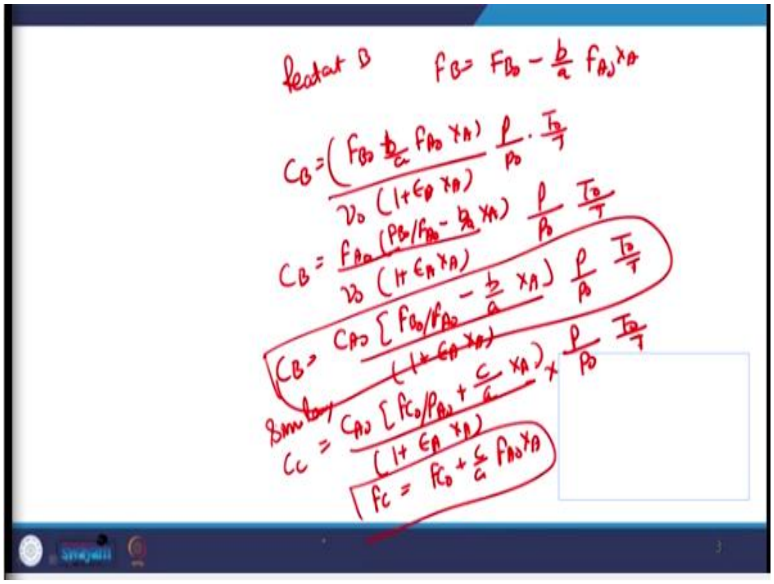
Now here 1 + epsilon A X_A P upon P_0 T_0 upon T. Now if we see about the reactant concentration A then C_A = F_{A0} 1 - X_A 1 + epsilon A X_A P_0 upon P T upon T_0 as we know that F_A = F_{A0} 1 - X_A. Now here then C_A = C_{A0} 1 - X_A upon 1 + epsilon A X_A and that becomes the P_0 T_0 upon T.

$$C_i = \frac{F_i}{\nu} = \frac{F_{io}\,(1 - X_A)}{\nu_o(1 + \varepsilon X_A)\left(\frac{P_o}{P}\right)\left(\frac{T}{T_o}\right)}$$

$$C_A = \frac{F_A}{\nu} = \frac{F_{Ao}\,(1 - X_A)}{\nu_o(1 + \varepsilon X_A)\left(\frac{P_o}{P}\right)\left(\frac{T}{T_o}\right)}$$

$$C_A = \frac{C_{Ao}\,(1 - X_A)}{(1 + \varepsilon X_A)}\left(\frac{P}{P_o}\right)\left(\frac{T_o}{T}\right)$$

(Refer Slide Time: 27:14)



Reactant B $F_B = F_{B0} - \frac{b}{a} F_{A0} X_A$

$$C_B = \frac{\left(F_{B0} - \frac{b}{a} F_{A0} X_A\right)}{v_0 (1 + \epsilon_A X_A)} \frac{P}{P_0} \cdot \frac{T_0}{T}$$

$$C_B = \frac{F_{A0} \left(F_{B0}/F_{A0} - \frac{b}{a} X_A\right)}{v_0 (1 + \epsilon_A X_A)} \frac{P}{P_0} \frac{T_0}{T}$$

$$\boxed{C_B = \frac{C_{A0} \left[F_{B0}/F_{A0} - \frac{b}{a} X_A\right]}{(1 + \epsilon_A X_A)} \frac{P}{P_0} \frac{T_0}{T}}$$

Similarly

$$C_C = \frac{C_{A0} \left[F_{C0}/F_{A0} + \frac{c}{a} X_A\right]}{(1 + \epsilon_A X_A)} \times \frac{P}{P_0} \frac{T_0}{T}$$

$$\boxed{F_C = F_{C0} + \frac{c}{a} F_{A0} X_A}$$

Now similarly if we wish to have this type of equation for reactant B. So, let put this thing in this way $F_B = F_{B0}$ - B upon A F_{A0} X_A, now C_B = b upon a F_{A0} X_A upon v_0 (1 + epsilon A X_A) P upon P_0 into T_0 upon T or C B = F_{A0} F_{B0} upon F_{A0} - b upon a X_A and this is 1 + epsilon A X_A. And P upon P_0 T_0 upon t or C_B = C_{A0} F_{B0}, all these things are with their usual interpretation b upon a X_A into (1 + epsilon A X_A P upon P_0 T_0 upon T.

$$F_B = F_{Bo} - \frac{b}{a} F_{A_O} X_A$$

$$\Rightarrow C_B = \frac{\left(F_{Bo} - \frac{b}{a} F_{A_O} X_A\right)}{\nu_o (1 + \varepsilon X_A) \left(\frac{P_o}{P}\right) \left(\frac{T}{T_o}\right)}$$

$$\Rightarrow C_B = \frac{F_{Ao}\ (F_{Bo}/F_{A_O} - \frac{b}{a} X_A)}{\nu_o (1 + \varepsilon X_A)} \left(\frac{P}{P_o}\right) \left(\frac{T_o}{T}\right)$$

$$\Rightarrow C_B = \frac{C_{Ao}\ (F_{Bo}/F_{A_O} - \frac{b}{a} X_A)}{(1 + \varepsilon X_A)} \left(\frac{P}{P_o}\right) \left(\frac{T_o}{T}\right)$$

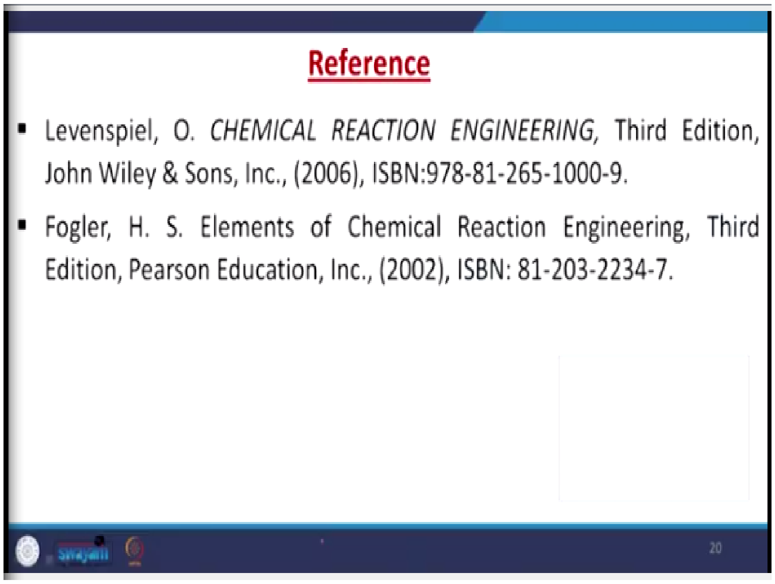
So, similarly we can write for concentration of C, this is C_{A0}. Now here we are putting the plus sign because the C is being generated in due course of time upon 1 + epsilon A X_A multiplied by P upon P_0 T_0 upon T. Now here $F_C = F_{Co}$ + c upon a F_{A0} X_A. So, by this way we generated these mathematical equations for prediction of varying volume concept. Now at last in this particular segment we discuss the varying volume concept and with the taking the concentration into cognizance. And we developed the various equation associated to this for the interpretation of batch reactor data.

$$\Rightarrow C_C = \frac{C_{Ao}\left(\frac{F_{Co}}{F_{A_O}} + \frac{c}{a}X_A\right)}{(1+\varepsilon X_A)}\left(\frac{P}{P_o}\right)\left(\frac{T_o}{T}\right)$$

As,

$$F_C = F_{Co} + \frac{c}{a}F_{A_O}X_A$$

(Refer Slide Time: 30:04)



Reference

- Levenspiel, O. *CHEMICAL REACTION ENGINEERING*, Third Edition, John Wiley & Sons, Inc., (2006), ISBN:978-81-265-1000-9.
- Fogler, H. S. Elements of Chemical Reaction Engineering, Third Edition, Pearson Education, Inc., (2002), ISBN: 81-203-2234-7.

Now if you wish to have further reading, again we have listed couple of references in their reference slide and hope that this particular lecture you enjoyed a lot, thank you very much.