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

Lecture – 14
Temperature Dependent Terms And Interpretation of Batch Reactor Data - I

Welcome to the next lecture of polymer reaction engineering. Here we are going to discuss with the various temperature dependent terms and interpretation of various kinds of batch reactor data. So, let us have a look about what we have studied previously. So, we had a discussion about various approaches of reactor design. What are the integral components involved in the reactor design? What are the rate laws? What are the different types of reactions? What are the rate equations? etc.

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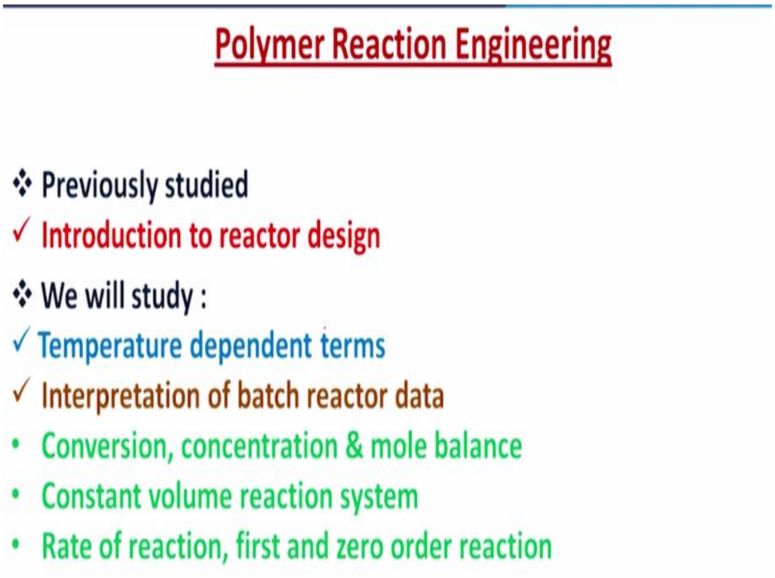

Polymer Reaction Engineering

❖ Previously studied
✓ Introduction to reactor design
❖ We will study :
✓ Temperature dependent terms
✓ Interpretation of batch reactor data
- Conversion, concentration & mole balance
- Constant volume reaction system
- Rate of reaction, first and zero order reaction

Now, in this lecture series we will discuss about the concept of temperature dependent term. We will interpret the various batch reactor data available during the course of time. We will have a brief outlook about the conversion, concentration and mole balance concepts. We will discuss about the system pertaining to the constant volume reaction approaches. And then again, we will come back to the rate of reaction.

Specially emphasizing to the first and zero order reaction those who are attributed to the polymer synthesis or polymer reaction. So, let us have first thing related to the temperature dependent term. Now as we agree upon that the temperature plays a very vital role in the reaction design or reactor design and there are so, many types of reactors which we had already discussed in the previous lecture and everywhere you find that the output is usually dependent on the temperature.

So, there are various laws they are embedded in this temperature dependent term. One is the Arrhenius law. It is a very well-known law and very common law. Now, this law suggests formula for the temperature dependency of any kind of reaction rates. So, we discussed these reaction rates in the previous lecture.

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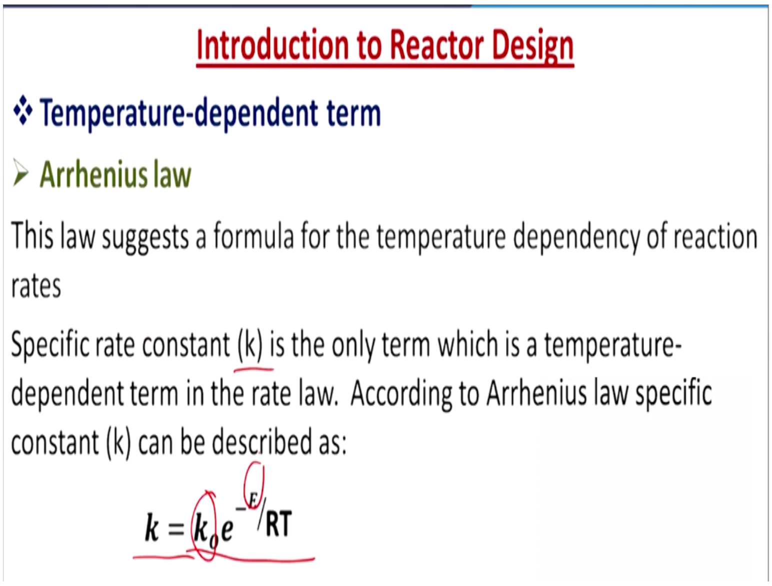

Introduction to Reactor Design

❖ Temperature-dependent term

➢ Arrhenius law

This law suggests a formula for the temperature dependency of reaction rates

Specific rate constant (k) is the only term which is a temperature-dependent term in the rate law. According to Arrhenius law specific constant (k) can be described as:

$$k = k_o e^{-E/RT}$$

Now, here this the temperature dependency is tutored by this Arrhenius law. Now, the integral part of this Arrhenius law that the specific rate constant usually denoted with the help of small k is the only term which is a temperature-dependent term in the rate law. So, according to Arrhenius law, the specific constant, whatever specific constant this can be defined as. We had already discussed this particular equation.

According to Arrhenius law we know

$$k = k_o e^{-E/\mathrm{RT}}$$

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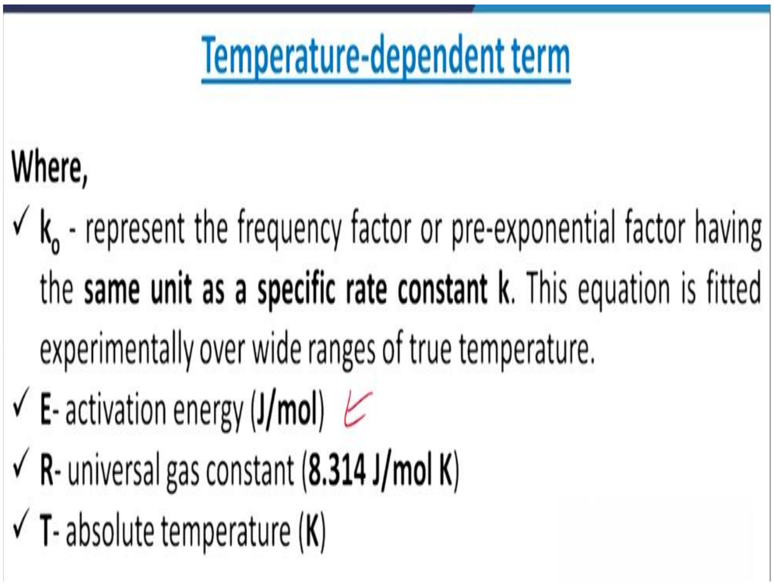

Temperature-dependent term

Where,

✓ k_0 - represent the frequency factor or pre-exponential factor having the **same unit as a specific rate constant k**. This equation is fitted experimentally over wide ranges of true temperature.

✓ **E**- activation energy (**J/mol**)

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

✓ **T**- absolute temperature (**K**)

Now, here in this previous equation k_0 represents the frequency factor or pre-exponential factor and having the same unit as the specific rate constant k. Now, this equation is fitted experimentally over a wide range of real temperature profile. Here this E is the activation energy and usually represented in the unit of joule per mole. R is the universal gas constant and the value is sometimes referred as 8.314 joule per mole Kelvin and T in this particular equation is the temperature, absolute temperature and represented as K that is kelvin.

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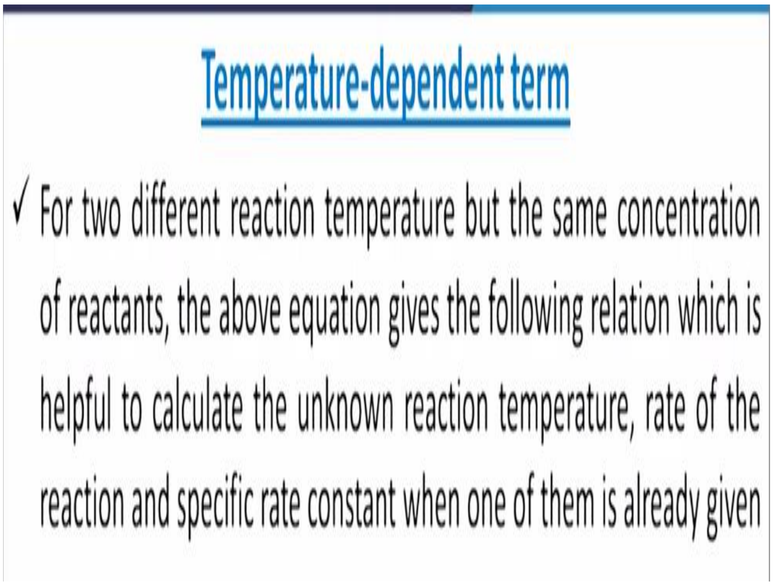

Temperature-dependent term

✓ For two different reaction temperature but the same concentration of reactants, the above equation gives the following relation which is helpful to calculate the unknown reaction temperature, rate of the reaction and specific rate constant when one of them is already given

Now for two different reaction temperature if they are having the same concentration of reactant, this equation gives a different type of equation which we are going to discuss, which is helpful to calculate unknown reaction temperature, rate of the reaction and a specific rate constant when one of them is usually given. So, let us have a look about this particular approach.

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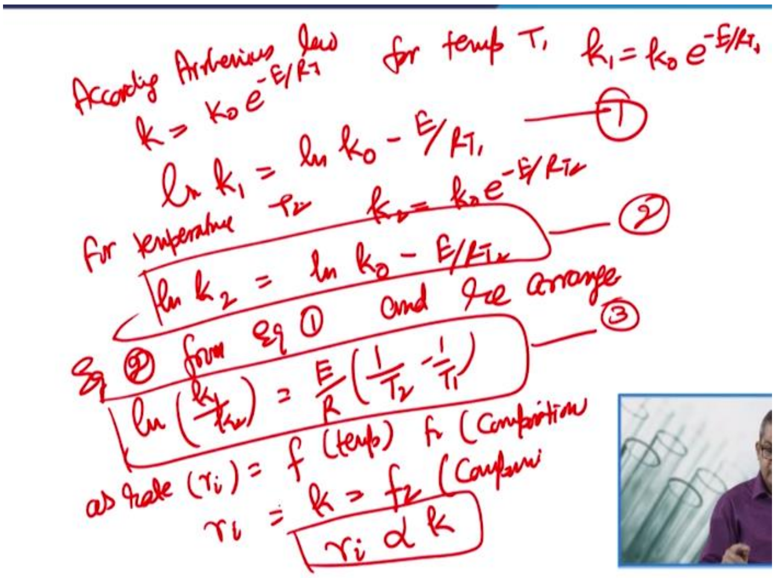

According Arrhenius law

$k = k_o e^{-E/RT}$

for temp T_1 $k_1 = k_o e^{-E/RT_1}$

$\ln k_1 = \ln k_o - E/RT_1$ — ①

for temperature T_2 $k_2 = k_o e^{-E/RT_2}$

$\boxed{\ln k_2 = \ln k_o - E/RT_2}$ — ②

Eq ② from Eq ① and re arrange

$\boxed{\ln\left(\frac{k_1}{k_2}\right) = \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$ — ③

as rate $(r_i) = f(\text{temp})\ f_2(\text{Composition}$

$r_i = k\ f_2(\text{Composi}$

$\boxed{r_i \propto k}$

Now according to Arrhenius law, we are having k = k_0 e to the power –E upon RT.

$$k = k_o e^{-E/\mathrm{RT}}$$

Now, for a temperature T_1, k_1 = k_0 e to the power –E/RT_1. Now if we take the log of both sides, then this equation becomes k_1 = lnk_0 – E upon RT_1. This is equation number 1 let us say.

$$\ln(\mathrm{k}_1) = \ln\mathrm{k}_\mathrm{o} - \frac{\mathrm{E}}{\mathrm{RT}_1}$$

Now for temperature T_2 this equation becomes k_2 = k_0 –E/RT_2. Now again if you take the log then this lnk_2 is k_0 –E/RT_2.

$$\ln(\mathrm{k}_2) = \ln\mathrm{k}_\mathrm{o} - \frac{\mathrm{E}}{\mathrm{RT}_2}$$

So, this is your equation number 2. Now if we subtract this equation 2 from equation 1 and if we rearrange the things, then we will have ln k_1 upon k_2 is equal to E/R into 1/T_2 – 1/T_1. This is equation number 3.

$$\ln\left(\frac{\mathrm{k}_1}{\mathrm{k}_2}\right) = \frac{\mathrm{E}}{\mathrm{R}}\left(\frac{1}{\mathrm{T}_2} - \frac{1}{\mathrm{T}_1}\right)$$

So, as rate say r_i is a function of, we have discussed this thing previously function of temperature, composition. So, r_i = kf_2 composition or r_i is proportional to k.

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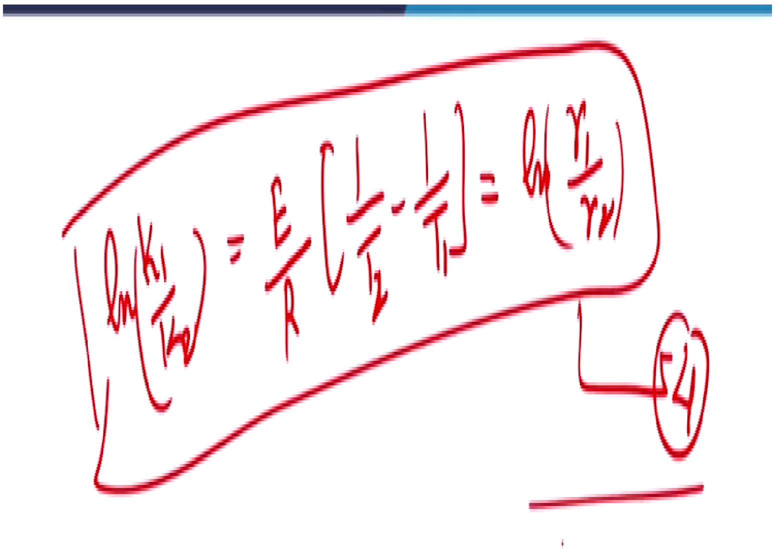

$$\boxed{\ln\left(\frac{k_1}{k_2}\right) = \frac{E}{R}\left[\frac{1}{T_2} - \frac{1}{T_1}\right] = \ln\left(\frac{r_1}{r_2}\right)}$$

(4)

So, therefore lnk_1 upon k_2 is referred as E upon R 1 upon T_2 –1 upon T_1r_1 upon r_2. So, this is you can say your master or generalized equation referred to as equation number 4.

$$\ln\left(\frac{k_1}{k_2}\right) = \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \ln\left(\frac{r_1}{r_2}\right)$$

Please try to remember this particular equation because we will utilize this equation thereafter.

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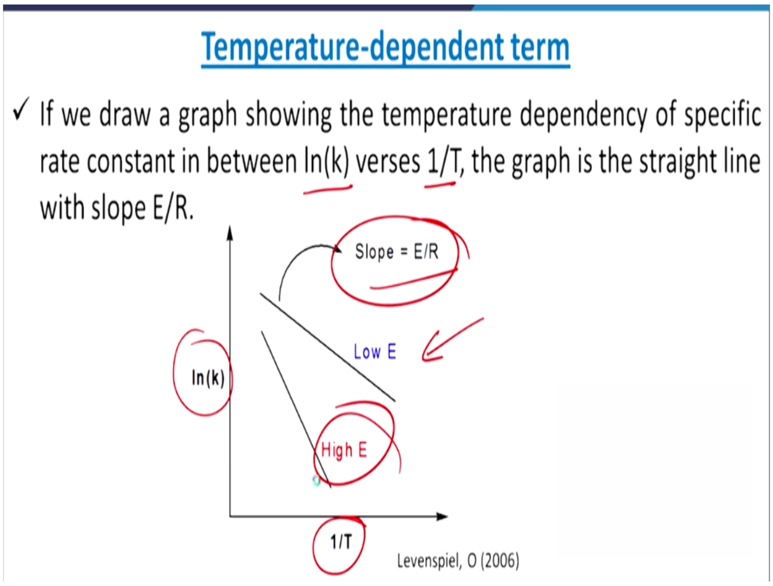

Temperature-dependent term

- ✓ If we draw a graph showing the temperature dependency of specific rate constant in between ln(k) verses 1/T, the graph is the straight line with slope E/R.

Levenspiel, O (2006)

So, now if we draw the graph showing the temperature dependency of a specific rate constant in between lnk versus 1 upon T, so usually the graph is a straight line with the slope of E upon R. So, here we have brought this one. Now if we are having the low activation energy, then the slope would be represented as E upon R and if we are having the high activation energy then it is represented like this.

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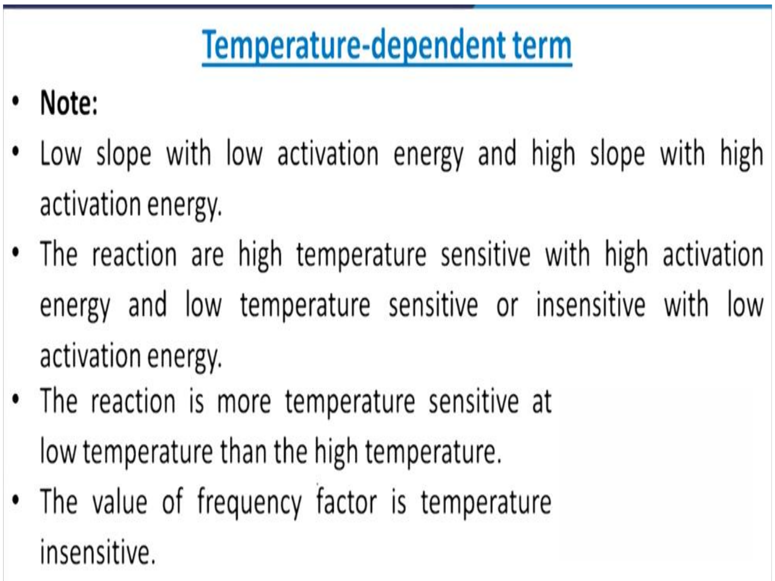

Temperature-dependent term

- **Note:**
- Low slope with low activation energy and high slope with high activation energy.
- The reaction are high temperature sensitive with high activation energy and low temperature sensitive or insensitive with low activation energy.
- The reaction is more temperature sensitive at low temperature than the high temperature.
- The value of frequency factor is temperature insensitive.

So, let us interpret this thing in a sequential order. Low slope with a low activation energy; this is the low slope with the low activation energy and it represents the high slope with high activation energy. So, the reactions are high temperature sensitive with the high activation energy and a low temperature sensitive or insensitive with low activation energy. The reactions are sometimes more temperature sensitive at low temperature then high temperature.

And the value of the frequency factor is sometimes temperature insensitive. Now, people try to develop this particular approach with the help of a collision theory which we discussed in the previous lecture.

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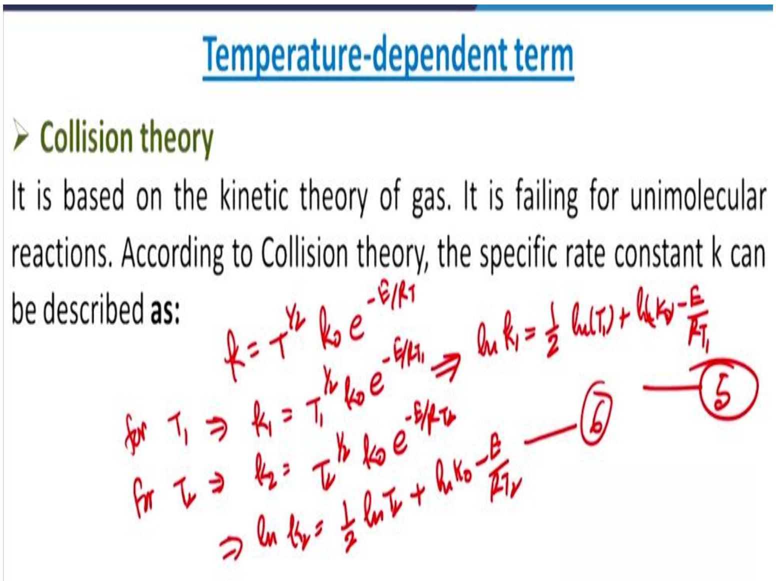

Temperature-dependent term

- **Collision theory**

It is based on the kinetic theory of gas. It is failing for unimolecular reactions. According to Collision theory, the specific rate constant k can be described **as:**

$$k = T^{1/2} k_0 e^{-E/RT}$$

$$\text{for } T_1 \Rightarrow k_1 = T_1^{1/2} k_0 e^{-E/RT_1} \Rightarrow \ln k_1 = \frac{1}{2}\ln(T_1) + \ln k_0 - \frac{E}{RT_1} \quad \text{—⑤}$$

$$\text{for } T_2 \Rightarrow k_2 = T_2^{1/2} k_0 e^{-E/RT_2}$$

$$\Rightarrow \ln k_2 = \frac{1}{2}\ln T_2 + \ln k_0 - \frac{E}{RT_2} \quad \text{—⑥}$$

It is usually based on the kinetic theory of a gas and it is failing for unimolecular reaction. Now according to the collision theory, the specific rate constant k you can always describe as k = T to the power half k_0 e –E upon RT. Now for say T_1 k_1 = T_1 half k_0 RT_1 or $\ln k_1$ = half $\ln T_1$ + ln k_0 –E upon RT_1. You may refer as equation number 5, previously we discussed the equation 4. For T_2 k_2 = T_2 RT_2 and ln T_2 + ln k_0 –E upon RT_2. This is equation number 6.

Equations

$$k = T^{1/2}\, k_o e^{-E/RT}$$

For temperature T_1

$$k_1 = {T_1}^{1/2}\, k_o e^{-E/RT_1}$$

Taking log both side we have

$$\ln k_1 = \frac{1}{2}\ln T_1 + \ln k_o - \frac{E}{RT_1}$$

For temperature T_2

$$k_2 = {T_2}^{1/2}\, k_o e^{-E/RT_2}$$

Taking log both side we have

$$\ln k_2 = \frac{1}{2}\ln T_2 + \ln k_o - \frac{E}{RT_2}$$

On subtracting above equations of two different temperature we have

$$\ln\left(\frac{k_1}{k_2}\right) = \ln\left(\frac{r_1}{r_2}\right) = \frac{1}{2}\ln\left(\frac{T_1}{T_2}\right) + \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

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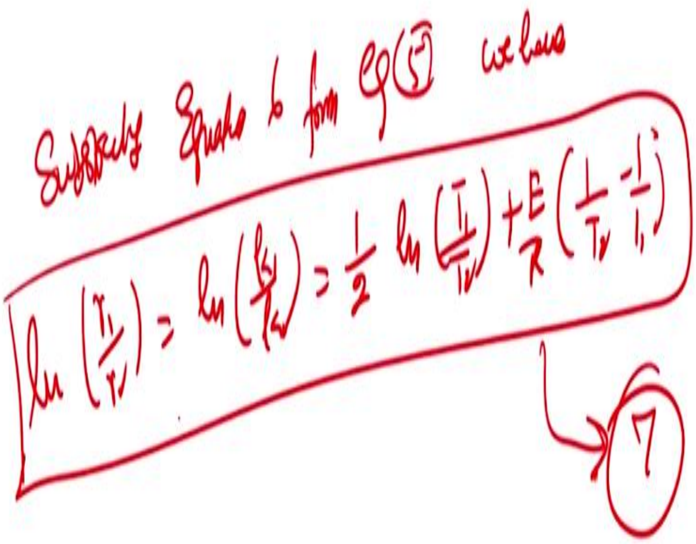

Subtracting Equation 6 from Eq (5) we have

$$\boxed{\ln\left(\frac{r_1}{r_2}\right) = \ln\left(\frac{k_1}{k_2}\right) = \frac{1}{2}\ln\left(\frac{T_1}{T_2}\right) + \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} \longrightarrow ⑦$$

Now, upon subtracting equation 6 from equation number 5 we have ln r_1 upon r_2 = $\ln k_1$ upon k_2 = 1 upon 2 $\ln T_1$ upon T_2 + E upon R into one upon T_2 – one upon T_1. Now, this is again the generalized equation and you may refer as equation number 7. So, by this way you can see that how this rate constant or a rate of a reaction depends on that temperature factor.

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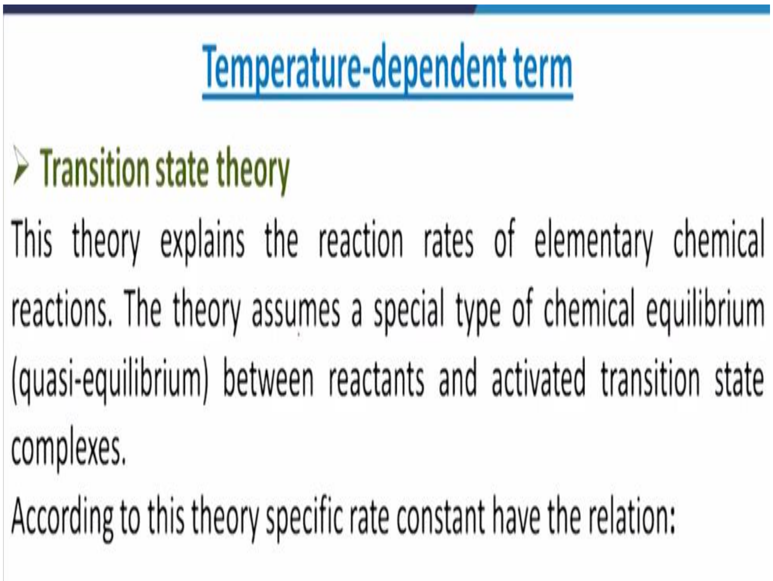

Temperature-dependent term

- Transition state theory

This theory explains the reaction rates of elementary chemical reactions. The theory assumes a special type of chemical equilibrium (quasi-equilibrium) between reactants and activated transition state complexes.

According to this theory specific rate constant have the relation:

Now, another theory which put forward to help the temperature dependency term that is called the transition state theory. Now, this theory particularly explains the reaction rate of elementary chemical reaction. If you recall that in the previous lecture we discussed about the elementary reactions. Now this theory assumes a special type of chemical equilibrium that is called the quasi-equilibrium.

This between the reactants and activation transition state complexes. Now according to this particular theory, the specific rate constant has the relations like this.

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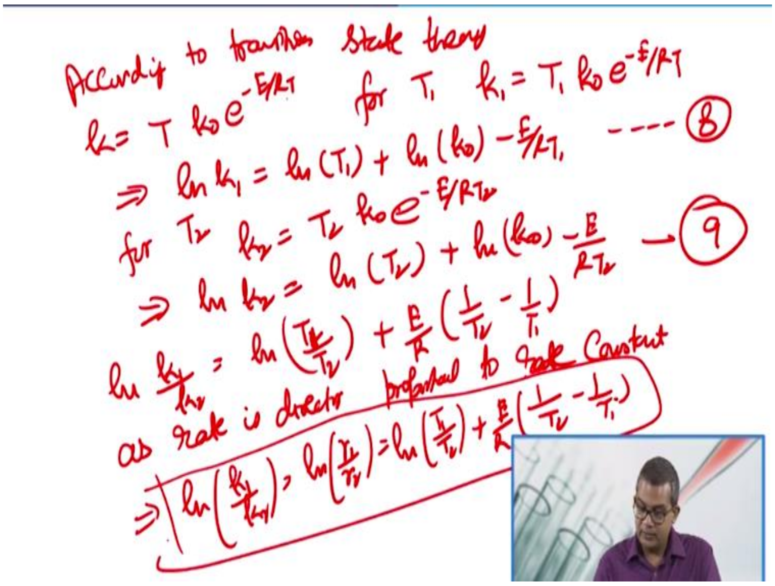

According to transition state theory

$k = T k_0 e^{-E/RT}$ for T_1 $k_1 = T_1 k_0 e^{-E/RT}$

$\Rightarrow \ln k_1 = \ln(T_1) + \ln(k_0) - E/RT_1$ ---- ⑧

for T_2 $k_2 = T_2 k_0 e^{-E/RT_2}$

$\Rightarrow \ln k_2 = \ln(T_2) + \ln(k_0) - \frac{E}{RT_2}$ → ⑨

$\ln \frac{k_1}{k_2} = \ln\left(\frac{T_1}{T_2}\right) + \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$

as rate is directly proportional to rate constant

$$\Rightarrow \boxed{\ln\left(\frac{k_1}{k_2}\right) = \ln\left(\frac{r_1}{r_2}\right) = \ln\left(\frac{T_1}{T_2}\right) + \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$$

Now, let us have a look about this relationship to transition state theory. Now k = T k_0 e upon minus E upon RT.

$$k = Tk_o e^{-E/RT}$$

For Temperature T_1

$$k_1 = T_1 k_o e^{-E/RT1}$$

Taking log both side we have

$$\ln k_1 = \ln T_1 + \ln k_o - \frac{E}{RT_1}$$

For Temperature T_2

$$k_1 = T_1 k_o e^{-E/RT2}$$

On taking log both side we have

$$\ln k_2 = \ln T_2 + \ln k_o - \frac{E}{RT_2}$$

Now for T_1 this $k_1 = T_1$ k_0 e to the power –E upon RT_2 or you say that $\ln k_1 = \ln T_1 + \ln k_0$ –E upon RT_1. Let us say this equation number 8. Now for T_2 $k_2 = T_2$ k_0, now remember our reactor operates in between T_1 and T_2. So, k_0 e to the power –E uponRT$_2$ or $\ln k_2 = \ln T_2 + \ln k_0$ –E upon RT_2. This is equation number 9.

On subtracting above two equations for two different temperature we have

$$\ln\left(\frac{k_1}{k_2}\right) = \ln\left(\frac{r_1}{r_2}\right) = \ln\left(\frac{T_1}{T_2}\right) + \frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Now, if we subtract this equation number 6 from 5, similarly we will have equation number 9 to 8, then we have $\ln k_1$ upon k_2 $\ln T_2$, sorry T_1, this is T_1 T_2 + E upon R. Now as rate is directly proportional to rate constant, this gives you $\ln k_1$ upon k_2 is equal to $\ln r_1$ upon r_2 is equal to $\ln T_1$ upon T_2 + E upon R_1 upon T_2 – 1 upon T_1. So, this is again one of the generalized equations and this we can say this is the equation number 10.

Now, sometimes we need to refer to the conversion aspect and this conversion aspect is again a very important part because ultimately decides the various factor attributed to the economics of the reactor, economics of your polymerization process.

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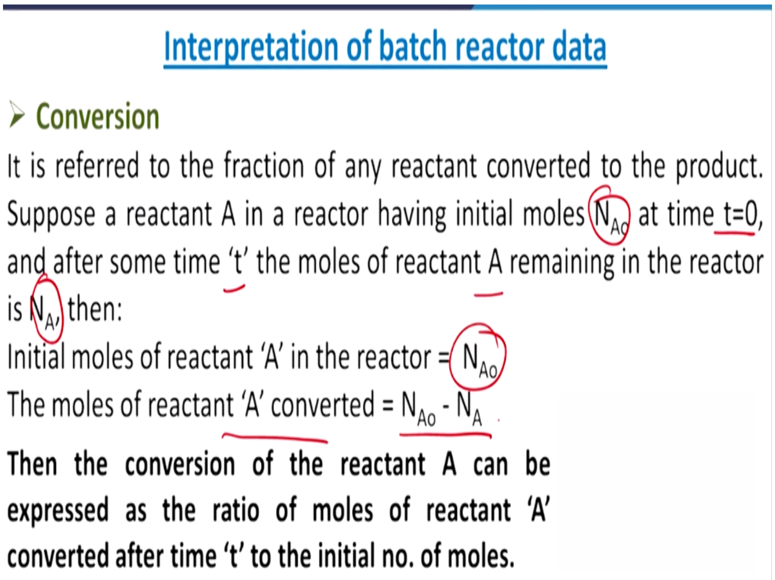

Interpretation of batch reactor data

- **Conversion**

It is referred to the fraction of any reactant converted to the product. Suppose a reactant A in a reactor having initial moles N_{Ao} at time t=0, and after some time 't' the moles of reactant A remaining in the reactor is N_A, then:

Initial moles of reactant 'A' in the reactor = N_{Ao}

The moles of reactant 'A' converted = $N_{Ao} - N_A$

Then the conversion of the reactant A can be expressed as the ratio of moles of reactant 'A' converted after time 't' to the initial no. of moles.

So, let us have a brief look about what is conversion. It is referred to the fraction of any reactant suppose A it is converted to the product and suppose reactant A in a reactor having initial moles of N_{A0} at time t = 0, that means at the startup and after some time t the moles of reactant A remaining the reactor are say N_A.

So, the initial moles of reactant A in the reactor N_{A0} and the moles of reactant A converted into product or any kind of a reaction they are $N_{A0} – N_A$. Now, then the conversion of reactant A can be expressed as the ratio of moles of reactant A converted after time t to the initial number of moles.

Conversion: It is referred to the fraction of any reactant converted to the product. Suppose a reactant A in a reactor having initial moles N_{Ao} at time t=0, and after some time t the moles of reactant A remaining in the reactor is N_A, then:

$$\text{The moles of reactant conveted} = \mathrm{N_{Ao}} - N_A$$

Initial moles of reactant in the reactor = N_{Ao}

Conversion can be expressed as the ratio of moles of reactant converted after time 't' to the initial no of moles. It is represented by X_A, for the conversion of reactant A.

$$\mathrm{X_A} = \frac{\mathrm{N_{Ao}} - \mathrm{N_A}}{\mathrm{N_{Ao}}}$$

$$\text{Moles of reactant A converted} = \mathrm{N_{Ao}} - \mathrm{N_A} = \mathrm{N_{Ao}X_A}$$

$$\text{Moles of reactant A remaining } (\mathrm{N_A}) = \mathrm{N_{Ao}}(1 - \mathrm{X_A})$$

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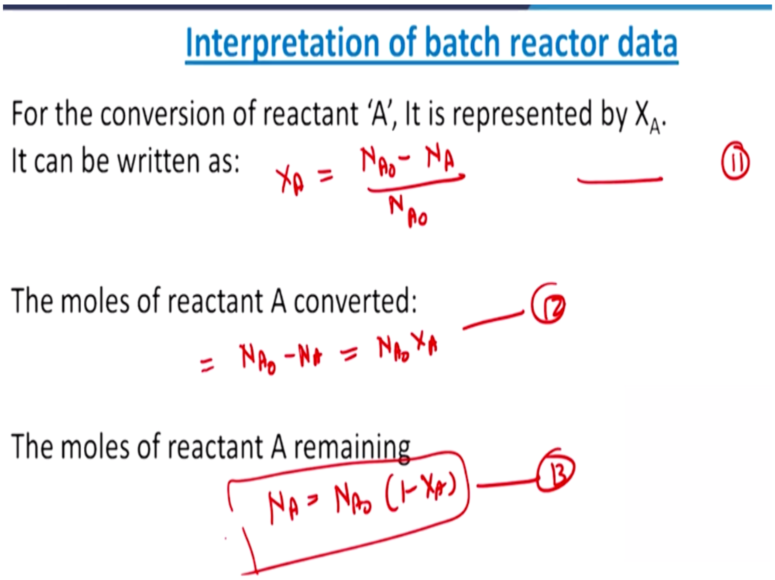

Interpretation of batch reactor data

For the conversion of reactant 'A', It is represented by X_A.

It can be written as: $X_A = \frac{N_{A0} - N_A}{N_{A0}}$ ⑪

The moles of reactant A converted: ⑫

$= N_{A0} - N_A = N_{A0}X_A$

The moles of reactant A remaining

$\boxed{N_A = N_{A0}(1-X_A)}$ ⑬

Now, sometimes mathematically we can represent this equation like this that is the conversion of reactant A that is sometimes referred as $X_A = N_{A0} - N_A$ upon N_{A0}. For reference we may site this equation as 11. Now, the most of reactant A converted and that is they are referred to as $N_{A0} - N_A = N_{A0}X_A$. And the most of reactant is remaining within the system they are N_{A0} into $1 - X_A$, this is referred as equation number 13.

Now, sometimes it gives you an important information pertaining to the unreacted segment of reaction mass that is why this particular information is extremely useful specifically for the separation process, specifically for the productivity, etc.

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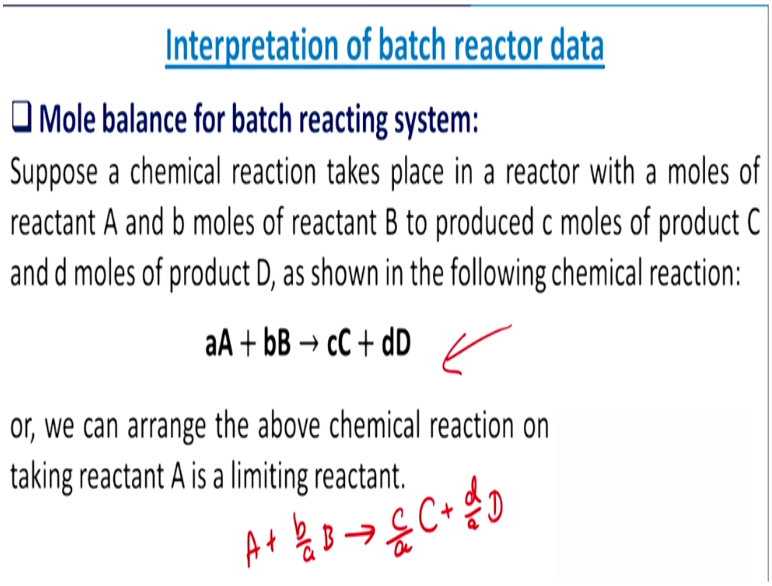

Interpretation of batch reactor data

❑ **Mole balance for batch reacting system:**

Suppose a chemical reaction takes place in a reactor with a moles of reactant A and b moles of reactant B to produced c moles of product C and d moles of product D, as shown in the following chemical reaction:

$$aA + bB \rightarrow cC + dD$$

or, we can arrange the above chemical reaction on taking reactant A is a limiting reactant.

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

Now, another thing which is important related to the interpretation of the batch reactor data that is the mole balance of a batch reacting system. Now suppose a chemical reaction takes place in a reactor with the moles of reactant A and B, right.

$$\mathrm{aA + bB \rightarrow cC + dD}$$

So, the corresponding you can say the stoichiometric number are small a and small b and by reacting with each other, they are forming the product C and D with their corresponding stoichiometric numbers c and d.

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

So, we can arrange this equation, which is the following equation on taking the reactant A as a limiting reactant and this equation can be modified as A + b upon a B c upon a C+ d upon a D.

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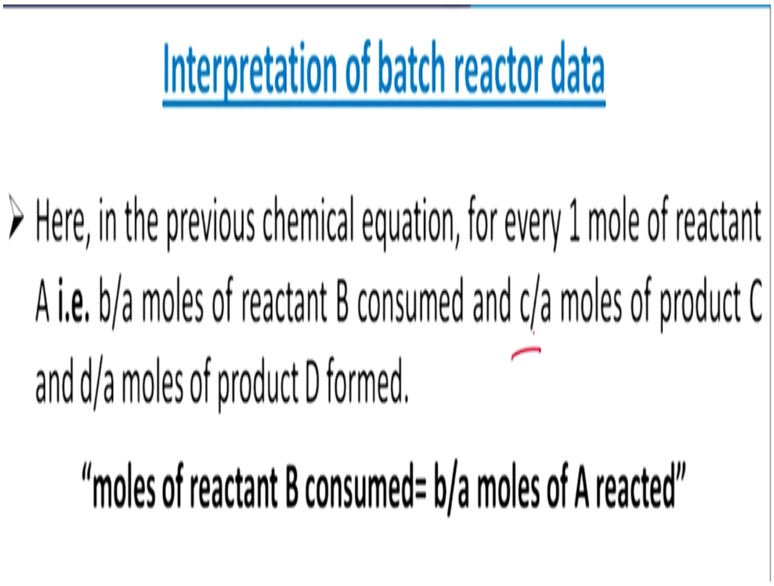

Interpretation of batch reactor data

- Here, in the previous chemical equation, for every 1 mole of reactant A **i.e.** b/a moles of reactant B consumed and c/a moles of product C and d/a moles of product D formed.

"moles of reactant B consumed= b/a moles of A reacted"

So, here the previous chemical equation, if you take the cognizance of the previous chemical equation for every one mole of reactant A, the b upon a mole of reactant B are consumed, that is why you need to put the negative sign over here and c upon a moles of product C and d upon a moles of product D are formed. So, usually you can say the moles of a reactant B consumed is equal to b upon a moles of A reacted.

$$\text{Moles of reactant A converted } = \mathrm{N_{Ao}} - N_A = N_{\mathrm{Ao}}X_A$$

$$\text{Moles of reactant A remaining } (N_A) = \mathrm{N_{Ao}}(1 - X_A)$$

$$\text{Moles of B reacted = b/a moles of A reacted}$$

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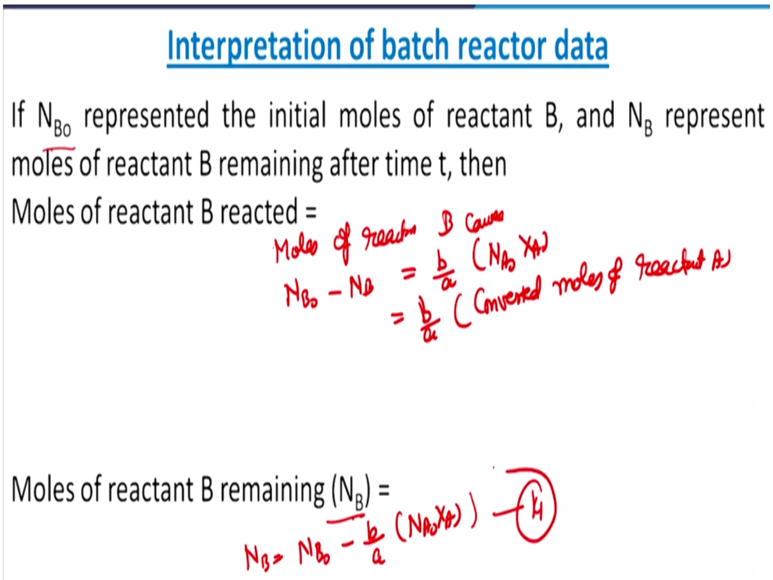

Interpretation of batch reactor data

If N_{Bo} represented the initial moles of reactant B, and N_B represent moles of reactant B remaining after time t, then

Moles of reactant B reacted =

Moles of reactan B Conv

$N_{Bo} - N_B = \frac{b}{a}(N_{Ao} X_A)$

$= \frac{b}{a}$ (Converted moles of reactant A)

Moles of reactant B remaining (N_B) =

$N_B = N_{Bo} - \frac{b}{a}(N_{Ao} X_A)$ — ⑭

Now if in other words we say that if N_{B0} this represents the initial moles of reactant B and N_B represents the moles of reactant B remaining after time t, with the help of this previous equation, you can represent that moles of reactant B converted that is $N_{B0} – N_B$ which is equal to b upon a $N_{A0}X_A$ or b upon a that is the converted moles of reactant A. So, the moles of reactant B remaining in the reaction mass that is represented as N_B.

This can be represented as $N_B = N_{B0} –$ b upon a $N_{A0}X_A$ and you can write this as equation number 14. Now because see when A and B both are consuming the reaction mass, then we have to look about the efficacy of the formation of product C and D for every mole of reactant A.

If N_{Bo} represented the initial moles of reactant B, and N_B represent moles of reactant B remaining after time t, then

$$\text{Moles of reactant B reacted} = N_{Bo} - N_B = b/a\ (N_{Ao}X_A)$$

$$\text{Moles of reactant B reacted} = N_{Bo} - N_B = \frac{b}{a}(N_{Ao}X_A)$$

or

$$N_B = N_{Bo} - \frac{b}{a}(N_{Ao}X_A)$$

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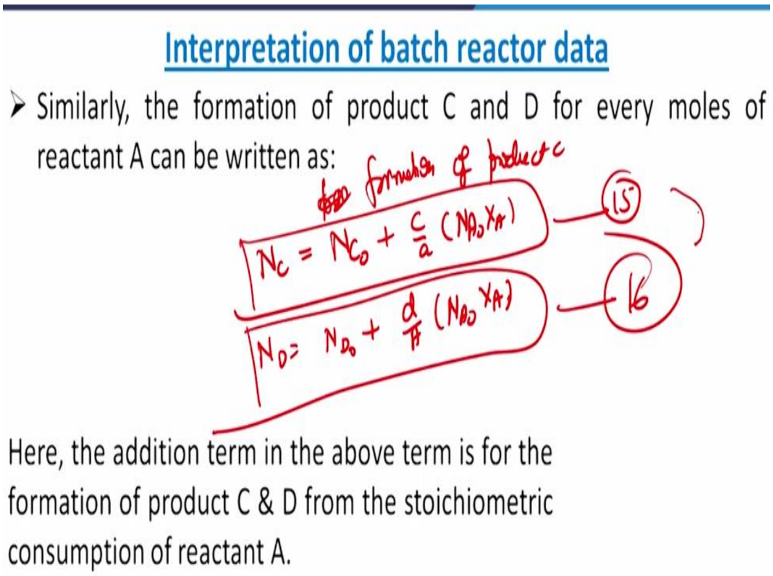

Interpretation of batch reactor data

- Similarly, the formation of product C and D for every moles of reactant A can be written as:

for formation of product C

$$N_C = N_{C_0} + \frac{c}{a}(N_{A_0}X_A) \quad (15)$$

$$N_D = N_{D_0} + \frac{d}{A}(N_{A_0}X_A) \quad (16)$$

Here, the addition term in the above term is for the formation of product C & D from the stoichiometric consumption of reactant A.

Now, this can be represented as the formation of the product C that is number of moles of C initially maybe if initially there is no mole of C present, then always you can put the numerical value equal to 0 plus c upon a $N_{A0}X_A$ that is the equation number 15. Now, similarly you can write for product D that is $N_D = N_{D0}$ + d upon a $N_{A0}X_A$. This is the equation number 16. Now, here the addition term in these two equations that is the formation of product C and D from the stoichiometric consumption of reactant A.

Similarly, for product C and D:

$$N_C = N_{\mathrm{Co}} + \frac{c}{a}(N_{\mathrm{Ao}}X_A)$$
$$N_D = N_{\mathrm{Do}} + \frac{d}{a}(N_{\mathrm{Ao}}X_A)$$

Here $\frac{c}{a}(N_{\mathrm{Ao}}X_A)$ moles of product C added to the initial moles of product C present and $\frac{d}{a}(N_{\mathrm{Ao}}X_A)$ moles of product D added to the initial moles of product D present initially.

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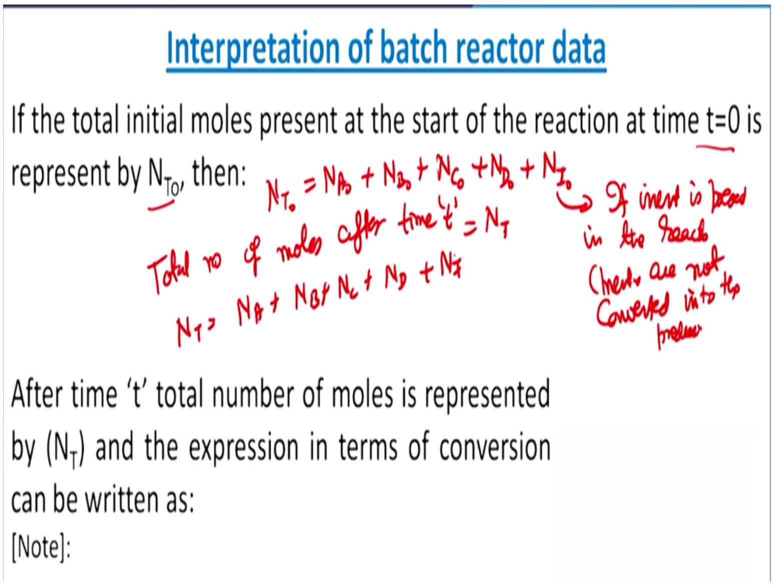

Interpretation of batch reactor data

If the total initial moles present at the start of the reaction at time t=0 is represent by N_{To}, then:

$N_{T_0} = N_{A_0} + N_{B_0} + N_{C_0} + N_{D_0} + N_{I_0}$ → If inert is present in the reactor (these are not converted into the product

Total no of moles after time 't' = N_T

$N_T = N_A + N_B + N_C + N_D + N_I$

After time 't' total number of moles is represented by (N_T) and the expression in terms of conversion can be written as:

[Note]:

Now if the total initial moles present at the start of the reaction at time t 0 = 0 is represented by N T0 then we can write this generalized equation $N_{T0} = N_{A0} + N_{B0} + N_{C0} + N_{D0} + N_{I0}$ this is if represented that if inert is present in the reactor. This is a very common thing, sometimes you need to put inert in the reactor to make the shift of reaction and these inerts are not converted into the product.

So, total number of moles at time t, moles after time t let us say they are equal to N_T. So, $N_T = N_A + N_B + N_C + N_D + N_I$.

Total initial number of moles present are N_{To} ($N_{To} = N_{Ao} + N_{Bo} + N_{Co} + N_{Do}$) and after time t total number of moles are N_T.

Where,

$$N_T = N_{To} + \delta(N_{Ao} X_A)$$

And $\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$ (Represent increase in total number of moles per unit moles of reactant A reacted)

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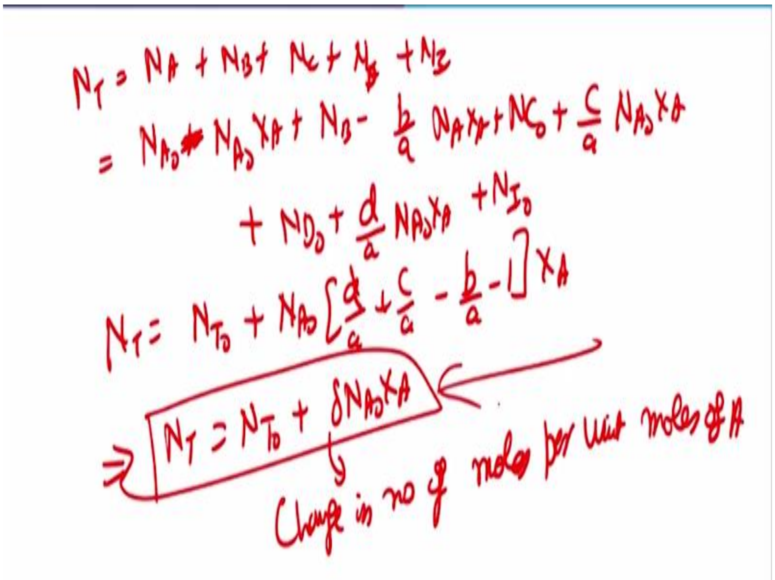

$$N_T = N_A + N_B + N_C + N_D + N_I$$

$$= N_{A0} - N_{A0}X_A + N_B - \frac{b}{a} N_A X_A + N_{C0} + \frac{c}{a} N_{A0} X_A$$

$$+ N_{D0} + \frac{d}{a} N_{A0} X_A + N_{I0}$$

$$N_T = N_{T0} + N_{A0}\left[\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right] X_A$$

$$\Rightarrow \boxed{N_T = N_{T0} + \delta N_{A0} X_A}$$

Change in no of moles per unit moles of A

Now if we expand this thing, then you can represent like this. Again I am writing back to this this equation $N_A + N_B + N_C$ just for the ease of explanation. Now this is N_{A0} +, sorry this is related to the consumption, so $N_{A0}X_A + N_B$ – b upon a $N_AX_A + N_{C0}$ + c upon a N_{A0} X_A N_{D0} + d upon a N_{A0} not X_A + N initial concentration. Now $N_T = N_{T0}N_{A0}$ not d upon a + c upon a – b upon a – 1 X_A.

Now this is $N_T = N_{T0}$ let us say that this is a change $N_{A0}X_A$. Now, this reflects the change in number of moles per unit moles of A. So, this particular equation is again a very crucial equation related to the conversion aspect and this is a very useful equation.

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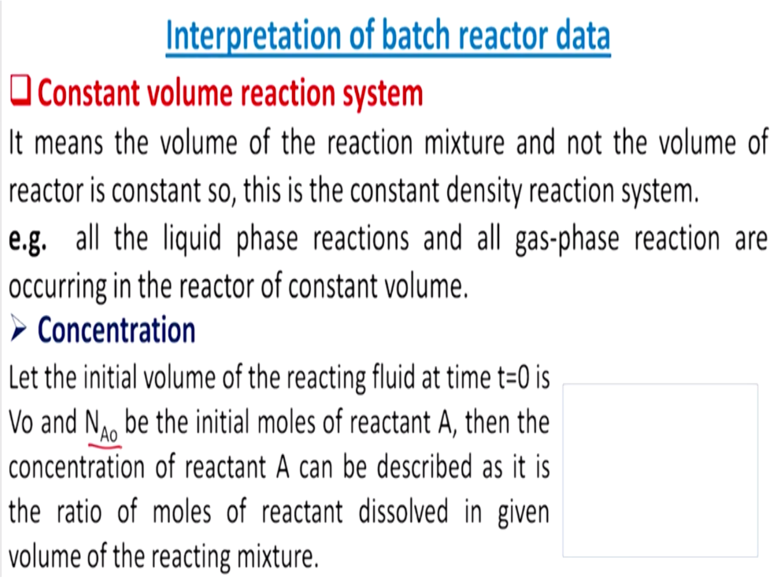

Interpretation of batch reactor data

☐ Constant volume reaction system

It means the volume of the reaction mixture and not the volume of reactor is constant so, this is the constant density reaction system.

e.g. all the liquid phase reactions and all gas-phase reaction are occurring in the reactor of constant volume.

- **Concentration**

Let the initial volume of the reacting fluid at time t=0 is Vo and N_{A0} be the initial moles of reactant A, then the concentration of reactant A can be described as it is the ratio of moles of reactant dissolved in given volume of the reacting mixture.

Let us have a brief look about the constant volume reaction system. Now, it means the volume of a reaction mixture and not the volume of the reactor is constant. So, that is the constant density reaction system. So, this relates to the constant density type of system like all fluid phase, all liquid phase reactions and all gaseous phase reactions are occurring in the reactor of constant volume.

Now, let us have a brief look about the concentration aspect in this kind of reaction system. Now, let the initial volume of reacting fluid at time $t_0 = 0$ be represented as V_0 and initial number of moles are N_{A0}. Then the concentration of the reactant A can be described as it is the ratio of moles of reactants those who are dissolved in a given volume of the reacting mixture.

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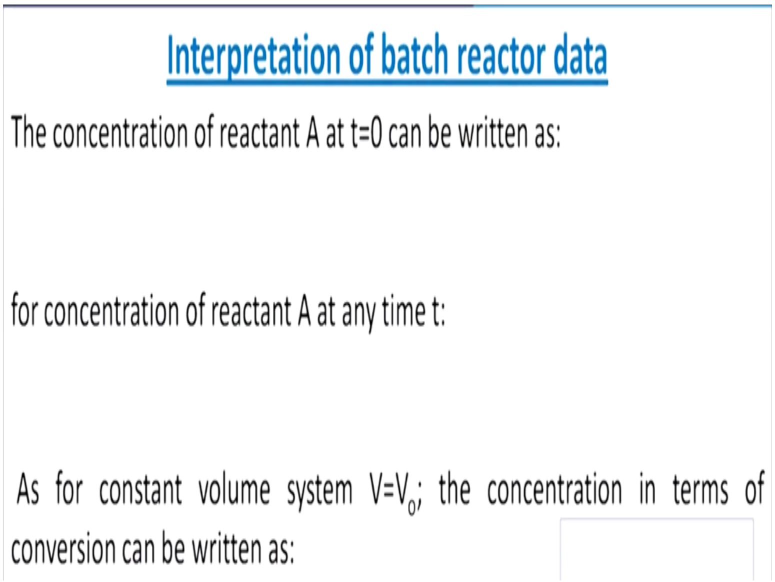

Interpretation of batch reactor data

The concentration of reactant A at t=0 can be written as:

for concentration of reactant A at any time t:

As for constant volume system $V=V_0$; the concentration in terms of conversion can be written as:

Now, this can be represented as the concentration of reactant A.

$$C_{\mathrm{Ao}} = \frac{N_{A_o}}{V_o}$$

for concentration of reactant A at any time t;

$$C_A = \frac{N_A}{V}$$

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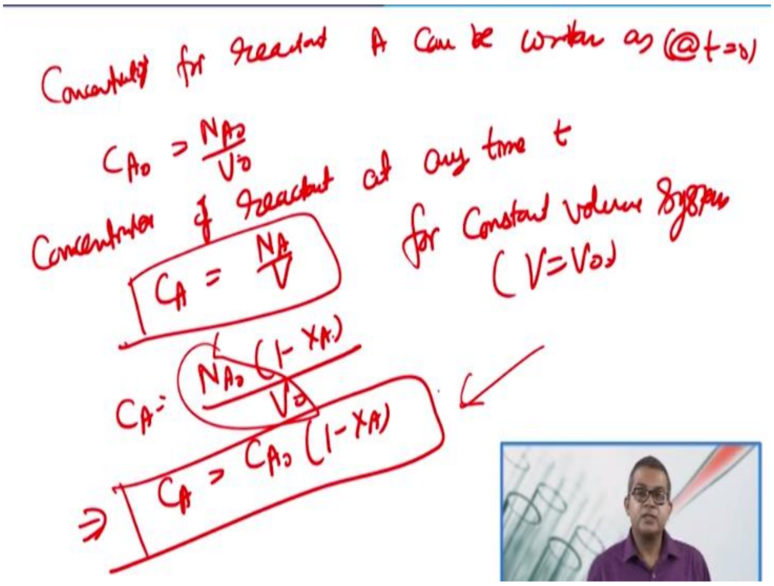

Concentration for reactant A can be written as (@t=0)

$$C_{A0} = \frac{N_{A0}}{V_0}$$

Concentration of reactant at any time t

$$\boxed{C_A = \frac{N_A}{V}}$$

for Constant volume System ($V=V_0$)

$$C_A = \frac{N_{A0}(1-X_A)}{V_0}$$

$$\Rightarrow \boxed{C_A = C_{A0}(1-X_A)}$$

The concentration for reactant A can be written as at t = 0 that is $C_{A0} = N_{A0}V_0$. Now the concentration of a reactant at any time t this is equal to C_AN_A upon V with status V previously. Now for constant volume system this $V = V_0$. So, $C_A = N_{A0}(1 – X_A)$ upon V_0 or $C_A = C_{A0}$ because this becomes this one concentration term $C_{A0}(1 – X_A)$. So, this equation represents the concentration of reactant A to the system.

As for constant volume system $V=V_o$;

$$C_A = \frac{N_{A_o}(1-X_A)}{V_o}$$

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

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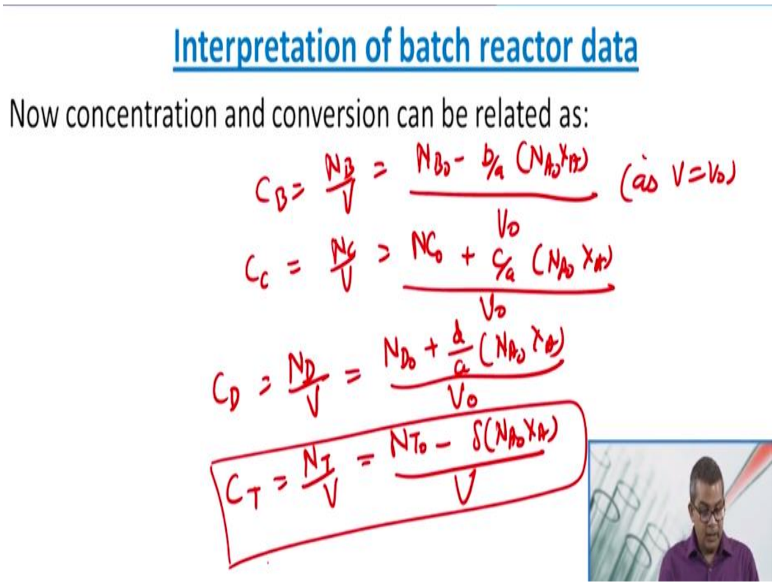

Interpretation of batch reactor data

Now concentration and conversion can be related as:

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - \frac{b}{a}(N_{A0}X_A)}{V_0} \quad (\text{as } V=V_0)$$

$$C_C = \frac{N_C}{V} = \frac{N_{C0} + \frac{c}{a}(N_{A0}X_A)}{V_0}$$

$$C_D = \frac{N_D}{V} = \frac{N_{D0} + \frac{d}{a}(N_{A0}X_A)}{V_0}$$

$$\boxed{C_T = \frac{N_T}{V} = \frac{N_{T0} - \delta(N_{A0}X_A)}{V}}$$

Now, the concentration and conversion these two things are very important related to the reactor data. Now, this can be clubbed or this can be related to each other like these equations.

So, let us have this particular approach C_B = N_B upon VN_{B0} – b upon a as V = V_0. Now concentration of C component that is N_C upon V = N_{C0} + c upon a.

C_D = concentration of component D is equal to and if we talk about a total concentration, then it can be represented as N_T upon V is N_{T0} $N_{A0}X_A$ upon V. So, these are the concentration conversion terms you can relate.

Similarly for the concentration terms for reactant B, product C and D can be written as follows;

On dividing each equation with volume of the reactor, we have

$$C_B = \frac{N_B}{V} = \frac{N_{Bo} - {}^{b}\!/_{a}\,(N_{Ao}X_A)}{V}$$

$$C_C = \frac{N_C}{V} = \frac{N_{Co} + {}^{c}\!/_{a}\,(N_{Ao}X_A)}{V}$$

$$C_D = \frac{N_D}{V} = \frac{N_{Do} - {}^{d}\!/_{a}\,(N_{Ao}X_A)}{V}$$

$$C_T = \frac{N_T}{V} = \frac{N_{To} - \delta(N_{Ao}X_A)}{V}$$

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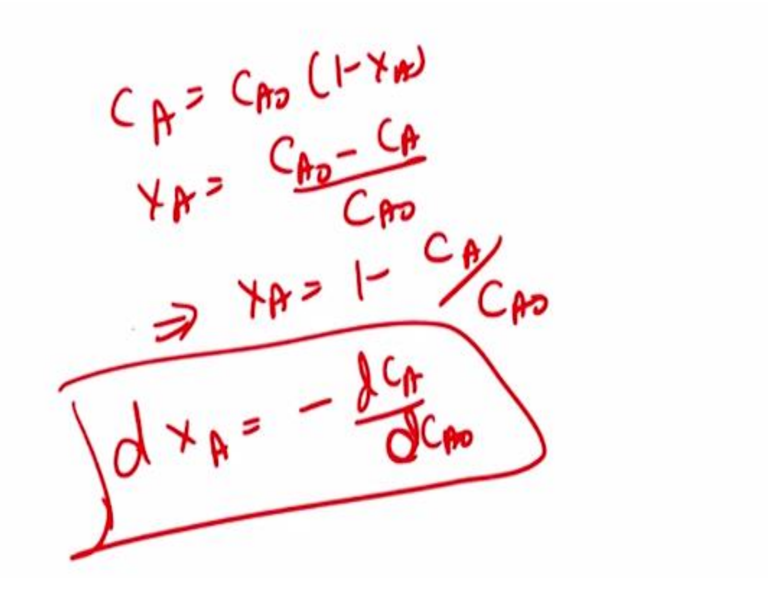

$$C_A = C_{A0}(1 - X_A)$$

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

$$\Rightarrow X_A = 1 - C_A/C_{A0}$$

$$\boxed{dX_A = -\frac{dC_A}{dC_{A0}}}$$

And to be more precise if we go if you go for this concentration conversion term again then C_A = $C_{A0}(1 – X_A)$, here X_A = C_{A0} – C_A upon C_{A0} or X_A = 1 – C_A upon C_{A0}. Now if we differentiate both side then it can be represented like –dC_A upon dC_{A0}. So, this is the generalized equation. So, in this particular lecture we discussed about the various factors associated with the interpretation of different kinds of a batch reactor data apart from other factors which are embedded for the designing of reactor concept.

Now concentration and conversion can be related as:

$$\Rightarrow \qquad X_A = \frac{C_{A_o} - C_A}{C_{A_o}}$$

$$\Rightarrow \qquad X_A = 1 - \frac{C_A}{C_{A_o}}$$

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

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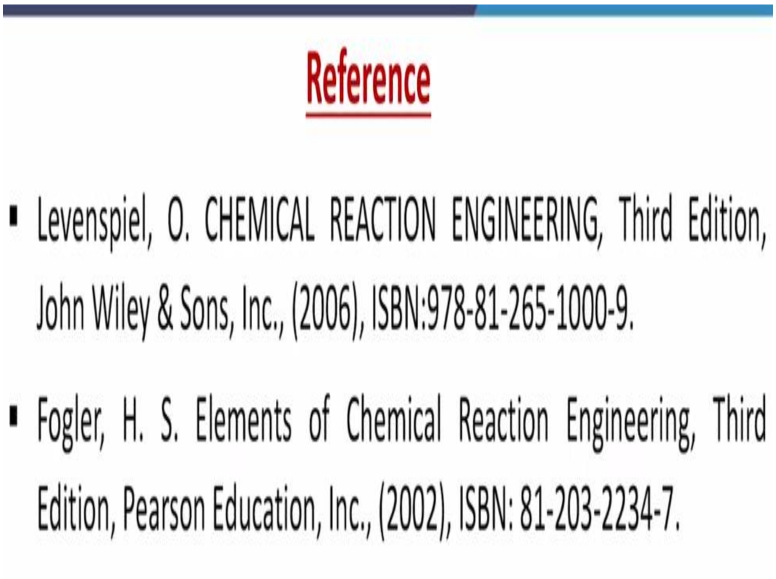

Reference

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Now by this way, I am summing up this particular lecture and we will continue about the rate of reaction and other parameters associated with the batch reactor design in the subsequent lecture. Thank you very much.