Chemical Reaction Engineering 1

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Lecture 12

Ideal Mixed Flow Reactor Design

Welcome to the second lecture of module 4. In this model we are discussing Reactor Design.

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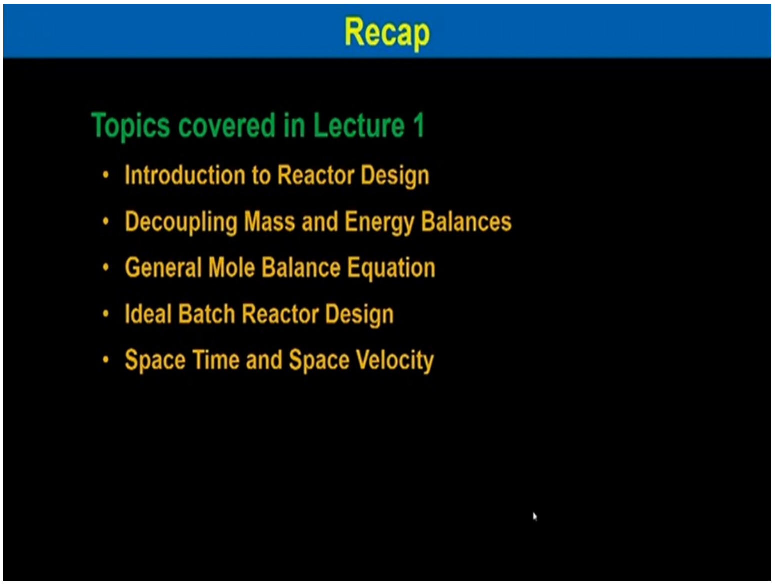

Recap

Topics covered in Lecture 1

- Introduction to Reactor Design
- Decoupling Mass and Energy Balances
- General Mole Balance Equation
- Ideal Batch Reactor Design
- Space Time and Space Velocity

Before going to this lecture let us have brief recap on our previous lecture. In lecture 1, we considered introduction to Reactor Design and we have considered what are the requirement to design a particular reactors. And then we have considered the concept of Decoupling of Mass and Energy Balance equations and with relevant examples of exothermic, highly exothermic, combustion reactions of methane in presence of oxygen.

And then we have considered general mole balance equation and taking into consideration this general mole balance equations we have tried to design ideal batch reactor. And then we have seen, what are the difference between the space time and the batch reactor time. So, we have discussed also space time and space velocity in lecture 1. Space time and space velocity these are natural measures for the flow reactors, whereas the time t in case of batch reactor is the natural measure for the performance of the batch reactor.

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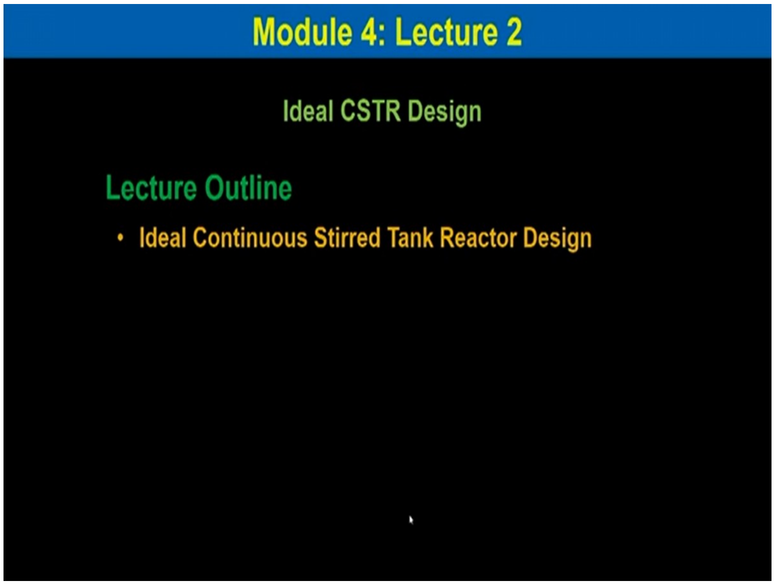

Module 4: Lecture 2

Ideal CSTR Design

Lecture Outline

- Ideal Continuous Stirred Tank Reactor Design

In this lecture, we will most concentrate on the design of ideal CSTR, CSTR means continuous stirred-tank reactor or it is a mixed flow reactor, so this is flow reactor it is used in different nomenclature in different books we can call it continuous stirred-tank reactor or as well as we can call it mixed flow reactor.

As we have said that for batch reactor we use only for the specialized applications when the quantity of the material to be processed is less or where we need to test a new product, so there we can use batch reactor or in case where the product or the reactant during the course of the reactions create scaling of the reactor in which we need to frequently clean the reactor in that case batch reactor is preferable, whereas for large scale industrial production usually we use the flow reactor. One of the flow reactor is CSTR continuous stirred-tank reactor and another reactor is the plug flow reactor.

So in this we will consider mostly ideal CSTR design. So the lecture's outline is we will discuss Ideal Continuous Stirred Tank Rector Design and we will see few examples to see how to calculate the different parameters for the continuous Stirred Tank Rector.

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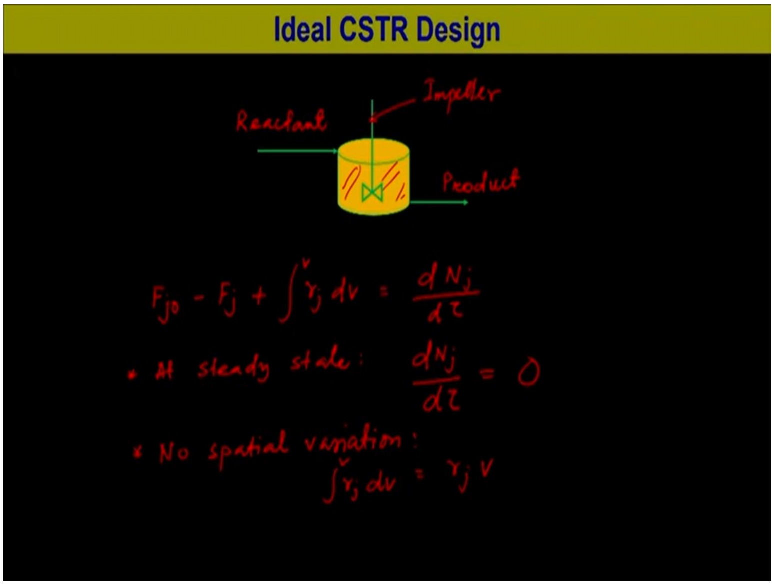

Ideal CSTR Design

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

- At steady state: $\frac{dN_j}{d\tau} = 0$
- No spatial variation: $\int^{V} r_j \, dv = r_j V$

So, let us consider ideal CSTR it is a tank fitted with impeller. So this is impeller and this is the inlet of the reactant and this is the product output. Now, we know the general mole balance equation say,

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

Now if we consider steady state, so at steady state what will happen, the change of mole with respect to time will be 0. That means here instead of dt we can write $d\tau$, for the flow reactor.

So at the steady state we can write $\frac{dN_j}{d\tau}$ is equal to 0 and if there is no special variation so for the case of no special variation that means it will not change in position so in that case the integral term we can write $\int^{V} r_j dV$ could be equal to $r_j V$. So, this is the case of for continuous Stirred Tank Reactor the reactant mixture is very well mixed in this region and they are homogeneous so there will not be any special variation of rate over this volume.

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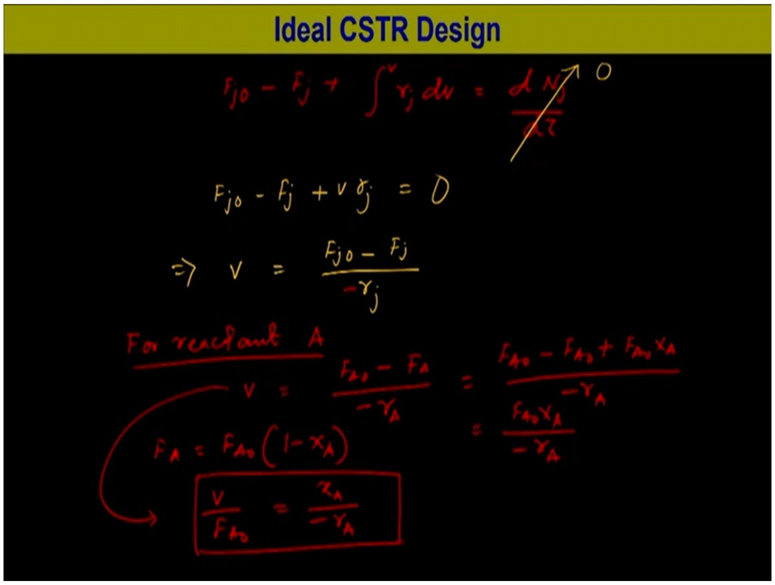

Ideal CSTR Design

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

$$F_{j0} - F_j + V r_j = 0$$

$$\Rightarrow V = \frac{F_{j0} - F_j}{-r_j}$$

For reactant A

$$V = \frac{F_{A0} - F_A}{-r_A} = \frac{F_{A0} - F_{A0} + F_{A0}X_A}{-r_A} = \frac{F_{A0}X_A}{-r_A}$$

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

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

Then the overall mole balance equation or general mole balance equation that is

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

So this is 0, so we can write

$$F_{j0} - F_j + Vr_j = 0$$

and if we rearrange we will get

$$V = \frac{F_j - F_{j0}}{r_j}$$

Now, if we write this equation for a particular species say for the reactant A, we can write

$$V = \frac{F_{A0} - F_A}{-r_A}$$

Now, if we substitute here

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

So this should be,

$$= \frac{F_{A0} X_A}{-r_A}$$

As you know

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

So form here we can write

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

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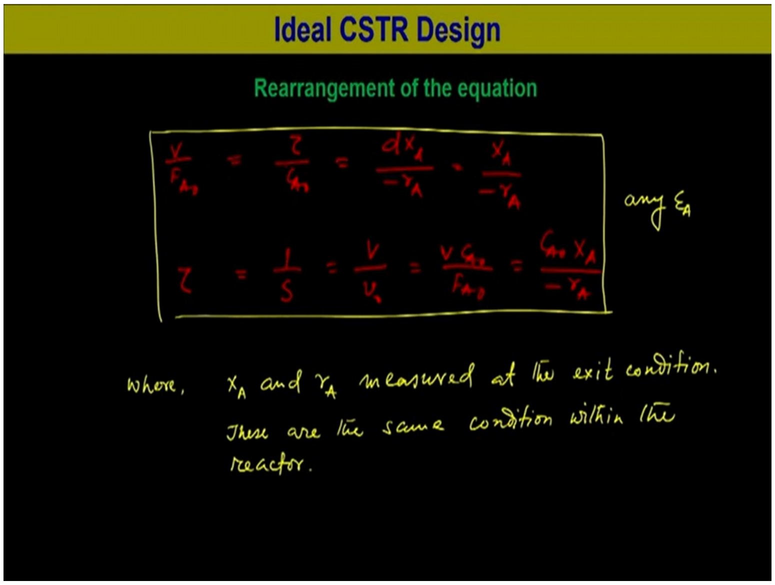

Ideal CSTR Design

Rearrangement of the equation

$$\boxed{\begin{array}{l}\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{dX_A}{-r_A} = \frac{X_A}{-r_A} \\ \tau = \frac{1}{S} = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}X_A}{-r_A}\end{array}}\quad \text{any } \varepsilon_A$$

where, X_A and r_A measured at the exit condition. These are the same condition within the reactor.

So now, if we rearrange this equation then we can write

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

or in other words we can write

$$\tau = \frac{1}{S} = \frac{V}{v_0}$$

We have done before the relations between the space time and space velocity would be equal to

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

So this relation after the rearrangement is valid for any ε_A and where X_A and r_A measured at the exit condition.

These are the same condition within the reactor. As we know for perfectly mixed flow reactor there is no special variation of the concentration so the concentration which we measure at the exit conditions should be same at the inside the reactor at any location at any time.

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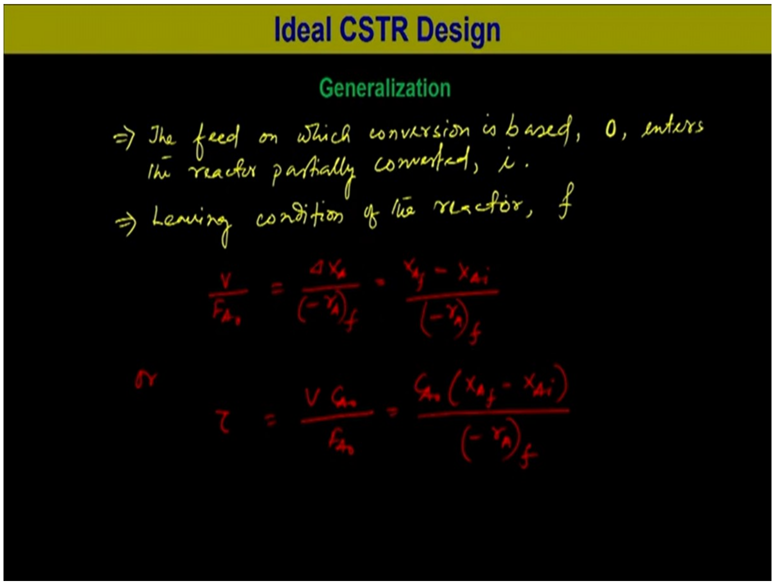

Ideal CSTR Design

Generalization

⇒ The feed on which conversion is based, 0, enters the reactor partially converted, i.

⇒ Leaving condition of the reactor, f

$$\frac{V}{F_{A0}} = \frac{\Delta X_A}{(-r_A)_f} = \frac{X_{Af} - X_{Ai}}{(-r_A)_f}$$

or

$$\tau = \frac{V C_{A0}}{F_{A0}} = \frac{C_{A0}(X_{Af} - X_{Ai})}{(-r_A)_f}$$

Now, if we generalize this relation and if we consider feed on which the conversion is based is entering conditions is represented with 0, that means the feed on which conversion is based if we represent with subscript 0, enter the reactor partially converted, then we represent with i and leaving conditions of the reactor is represented by f.

So entering conditions if it is partially converted which was represented with 0 earlier is represented by i and the leaving conditions of reactor which is the final is represented with f then the earlier equations we can write

$$\frac{V}{F_{A0}} = \frac{\Delta X_A}{-r_A} = \frac{X_{Af} - X_{Ai}}{-r_A}$$

And

$$\tau = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}(X_{Af} - X_{Ai})}{(-r_A)_f}$$

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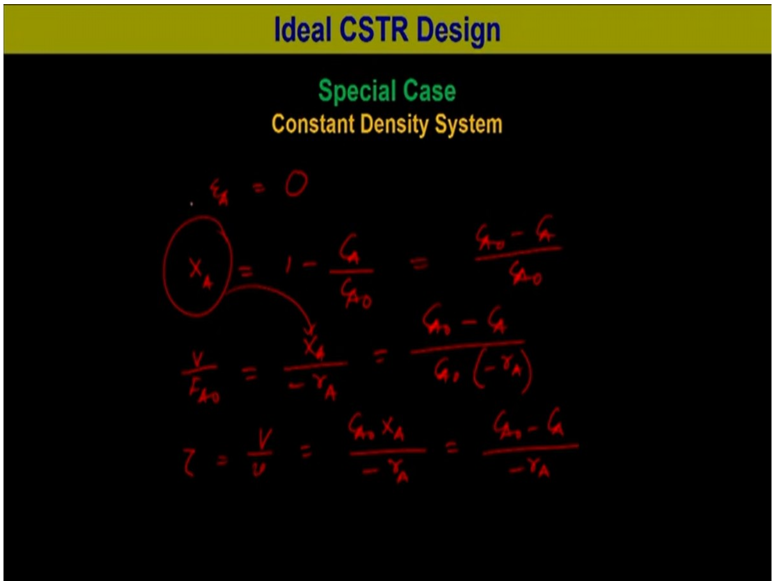

Ideal CSTR Design

Special Case

Constant Density System

$$\varepsilon_A = 0$$

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

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0}(-r_A)}$$

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

Now, if we consider special case for constant density system. So, if it is constant density system that means ε_A is equal to 0. So, the conversion can be related

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

then we can write

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0}(-r_A)}$$

So if we substitute

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

So if we substitute X_A from here in this, so we will have this relation or we can write

$$\tau = \frac{V}{v_0} = \frac{C_{A0} X_A}{-r_A} = \frac{C_{A0} - C_A}{-r_A}$$

So, this is for the special case of constant density system.

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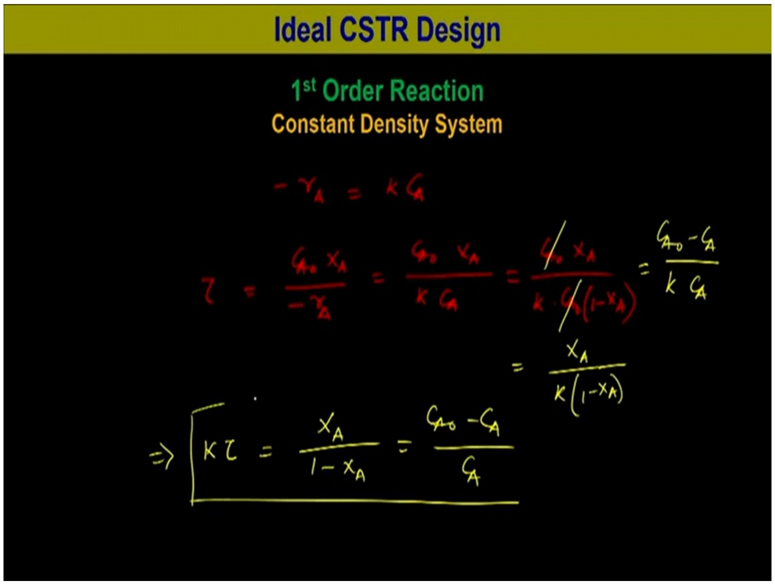

Ideal CSTR Design

1st Order Reaction

Constant Density System

$$-r_A = kC_A$$

$$\tau = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0}X_A}{kC_A} = \frac{\cancel{C_{A0}}X_A}{k\cancel{C_{A0}}(1-X_A)} = \frac{C_{A0}-C_A}{kC_A}$$

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

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

Now, if we consider first order reaction and it is for constant density system, then we can take first order example, the rate would be

$$-r_A = kC_A$$

Now

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

So, if we substitute this would be equal to

$$= \frac{C_{A0}X_A}{kC_A} = \frac{C_{A0}X_A}{kC_{A0}(1-X_A)}$$

So this C_{A0}, this would cancel out and we will have

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

So this can also be written as

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

So now, we can write

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

So this is for the first order constant density system.

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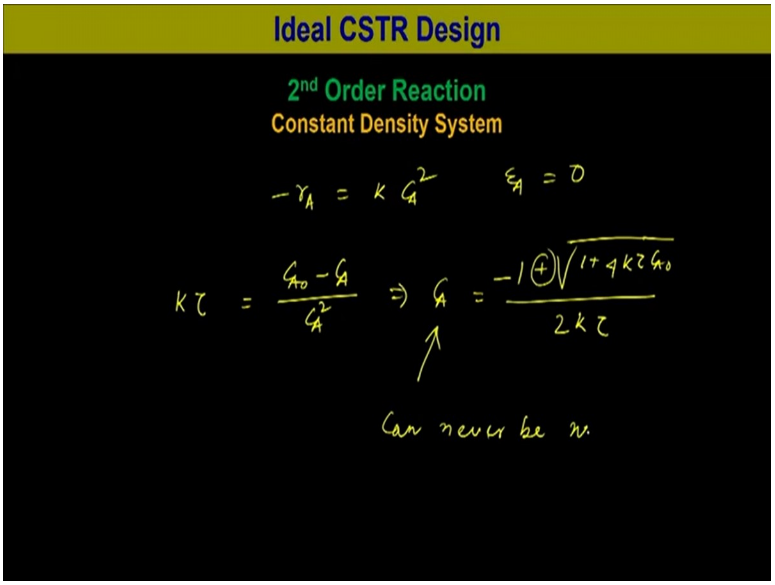

Ideal CSTR Design

2nd Order Reaction

Constant Density System

$-r_A = k C_A^2 \qquad \varepsilon_A = 0$

$k\tau = \frac{C_{A0} - C_A}{C_A^2} \Rightarrow C_A = \frac{-1 \oplus \sqrt{1 + 4k\tau C_{A0}}}{2k\tau}$

$\uparrow$

Can never be nv.

Now, if we consider second order constant density system it would be

$$-r_A = kC_A^2$$

And ε_A is equal to 0 constant density system so the $k\tau$ equations for the second order reaction

$$k\tau = \frac{C_{A0} - C_A}{C_A^2}$$

So from here we can write

$$C_A = \frac{-1 + \sqrt{1 + 4k\tau C_{A0}}}{2k\tau}$$

So this is only taken the positive part as you know the concentration can never be negative.

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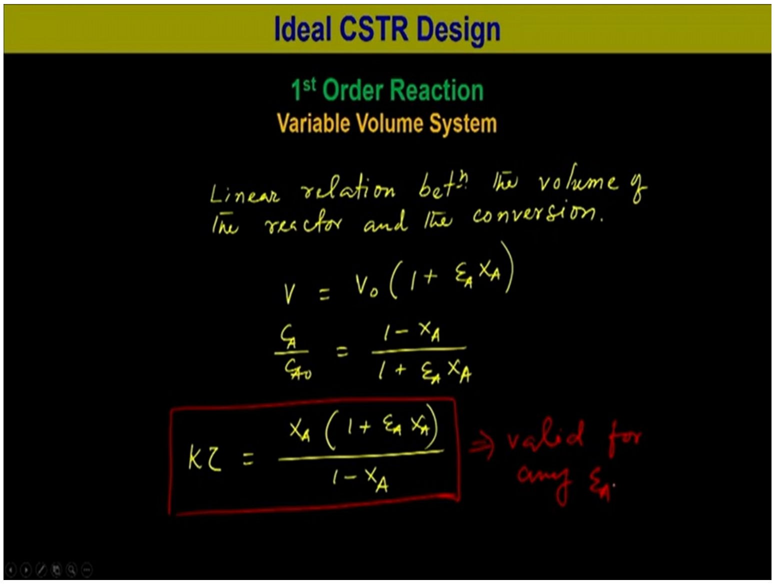

Ideal CSTR Design

1st Order Reaction

Variable Volume System

Linear relation betn the volume of the reactor and the conversion.

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

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

$$\boxed{k\tau = \frac{X_A(1+\varepsilon_A X_A)}{1-X_A}} \Rightarrow \text{valid for any } \varepsilon_A.$$

Now, if we consider first order reactions and variable volume system, in that case we can write there is linear relation between the volume and the conversions. So, linear relation the volume of the reactor and the conversion, so we can write

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

or

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

Now, the equations for

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

So this is relation for first order variable volume system is valid for any epsilon.

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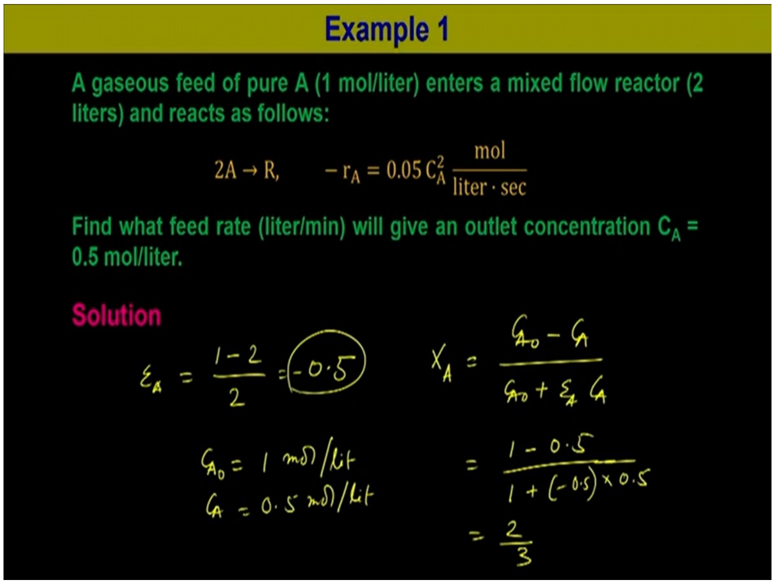

Example 1

A gaseous feed of pure A (1 mol/liter) enters a mixed flow reactor (2 liters) and reacts as follows:

$$2A \rightarrow R, \qquad -r_A = 0.05\,C_A^2 \,\frac{\text{mol}}{\text{liter} \cdot \text{sec}}$$

Find what feed rate (liter/min) will give an outlet concentration C_A = 0.5 mol/liter.

Solution

$$\varepsilon_A = \frac{1-2}{2} = \boxed{-0.5} \qquad X_A = \frac{C_{A0}-C_A}{C_{A0}+\varepsilon_A C_A}$$

$C_{A0} = 1$ mol/lit

$C_A = 0.5$ mol/lit

$$= \frac{1-0.5}{1+(-0.5)\times 0.5}$$

$$= \frac{2}{3}$$

Now, let us take an example how to calculate the parameters for the continuous stirred tank reactor design. A gaseous feed of pure A 1 mole per liter enters a mixed flow reactor having volume 2 liters and reacts as follows. So this is the reactions

$$2A \rightarrow R$$

Where rate is reaction is given,

$$-r_A = 0.05 C_A^2 \frac{mol}{liter.sec}$$

So this is second order reactions from the rate equations which is given and we need to find out what feed rate that is in liter per minute will give an outlet concentration that is C_A is 0.5 mole per liter.

So it started with pure A and we have the exit concentration which is given 0.5 mole per liter, so we have to find out the feed rate required for a stirred tank or mixed flow reactor. So let us solve it, if we evaluate the term first thing we have to do is the evaluation of the ε that is the change in volume that is fractional change that is

$$\varepsilon_A = \frac{1-2}{2}$$

so as we can see from the stoichiometric two moles of A reacts to produce one mole of r, so

$$\frac{1-2}{2} = -0.5$$

Now, as it is second order reactions, we know the relations between the conversion and the concentration, so

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

Now if we put the values that is C_{A0} is given 1 mole per liter C_A is given 0.5 mole per liter and ε_A is evaluated here, so if we put over here this would be

$$= \frac{1-0.5}{1+(-0.5)*0.5}$$

so this would be

$$= \frac{2}{3}$$

So, we have calculated X_A.

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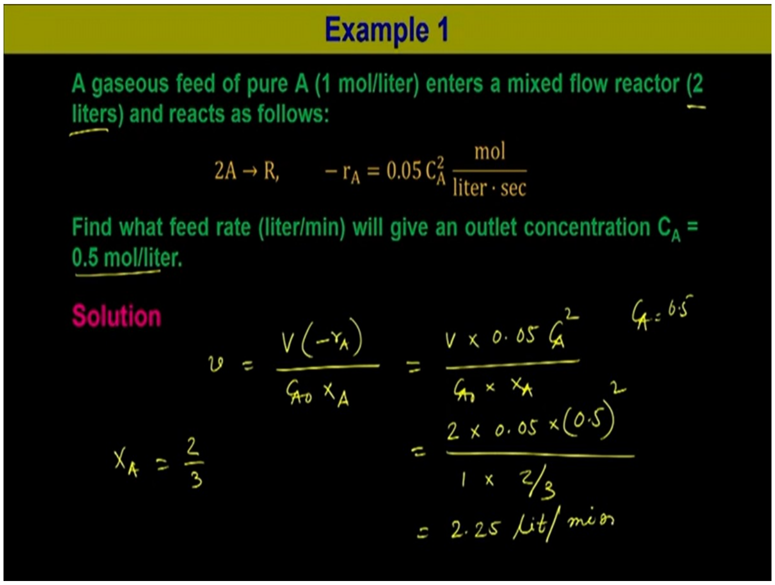

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Find what feed rate (liter/min) will give an outlet concentration C_A = 0.5 mol/liter.

Solution

$C_A = 0.5$

$$v = \frac{V(-r_A)}{C_{A0} X_A} = \frac{V \times 0.05\, C_A^2}{C_{A0} \times X_A}$$

$$X_A = \frac{2}{3}$$

$$= \frac{2 \times 0.05 \times (0.5)^2}{1 \times 2/3}$$

$$= 2.25 \text{ lit/min}$$

And now if we use the design equation for the CSTR we can write the volumetric flow rate or the feed rate v would be

$$v = \frac{V(-r_A)}{C_{A0}X_A}$$

Now, if we substitute the rate equations which is given over here, which is

$$= \frac{V * 0.05C_A^2}{C_{A0}X_A}$$

Now, if we substitute the values

$$= \frac{2 * 0.05 * (0.5)^2}{1 * 2/3}$$

So if we calculate the volumetric flow rate would be

$$= 2.25 lit/\min$$

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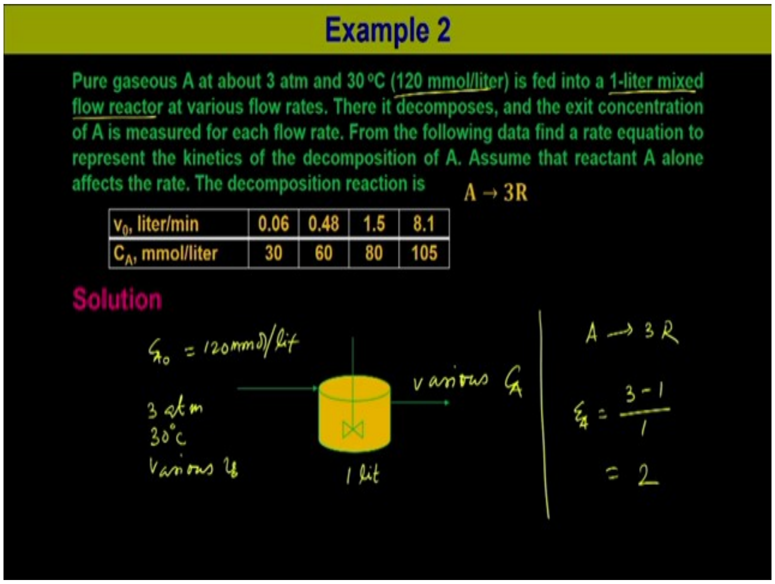

Example 2

Pure gaseous A at about 3 atm and 30 °C (120 mmol/liter) is fed into a 1-liter mixed flow reactor at various flow rates. There it decomposes, and the exit concentration of A is measured for each flow rate. From the following data find a rate equation to represent the kinetics of the decomposition of A. Assume that reactant A alone affects the rate. The decomposition reaction is $A \rightarrow 3R$

v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105

Solution

Let us take another example to calculate the kinetics of the reactions in a CSTR. A pure gas A at about 3 atmosphere and 30 degree centigrade, 120 millimole per liter is fed into a 1 liter mixed flow reactor at various flow rates. There it decomposes, and the exit concentration of A is measured for each flow rate. From the following data which is given over here, the volumetric flow rate and the concentration. So, different volumetric flow rates are given from the following data find a rate equation to represent the kinetics of the decomposition of A.

Assume that the reactant A alone affects the rate. So the decomposition reactions is given

$$A \rightarrow 3R$$

and it is said that reactant A alone affects the rate of rate of reactions, this is the problem now let us solve it. So this is a continuous Stirred tank reactor. So concentration of A C_{A0} the initial concentration is given 120 millimole this is the concentration. So, 120 mili mole per liter condition 3 atmosphere ,30 degree centigrade at various volumetric flow rate, v_0.

Volume of the reactor which is given 1 liter mixed flow reactor. So this is 1 liter and concentration coming out is various C_A. Now the reactions which is taking place that is

$$A \rightarrow 3R$$

for this we can calculate the change in volume this is gas phase reaction. So,

$$\varepsilon_A = \frac{3-1}{1} = 2$$

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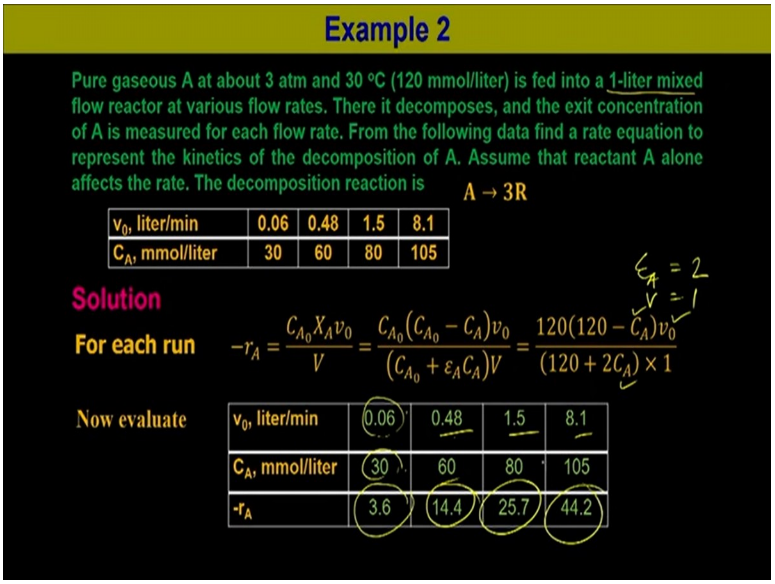

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v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105

Solution

$\varepsilon_A = 2$

$V = 1$

For each run $-r_A = \frac{C_{A_0} X_A v_0}{V} = \frac{C_{A_0}(C_{A_0} - C_A) v_0}{(C_{A_0} + \varepsilon_A C_A) V} = \frac{120(120 - C_A) v_0}{(120 + 2C_A) \times 1}$

Now evaluate

v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105
$-r_A$	3.6	14.4	25.7	44.2

So now, for each run we need to calculate the rate

$$-r_A = \frac{C_{A0} X_A \mathrm{v}_0}{V} = \frac{C_{A0}(C_{A0} - C_A)\mathrm{v}_0}{(C_{A0} + \varepsilon_A C_A)V}$$

So if we substitute the values so

$$-r_A = \frac{120(120 - C_A)\mathrm{v}_0}{(C_{A0} + 2C_A)1}$$

So for each run we can calculate based on this data volumetric flow rate for each volumetric flow rate we have concentration C_A at different volumetric flow rate so we can calculate substitute volumetric flow rate and concentration and calculate rate. So now, we can evaluate the rate at every conditions. So, this is for the volumetric flow rate of this 1 and this 1 so we can calculate if we substitute these two over here and we can get $-r_A$ is 3.6 and hence for every condition we can calculate the values of $-r_A$.

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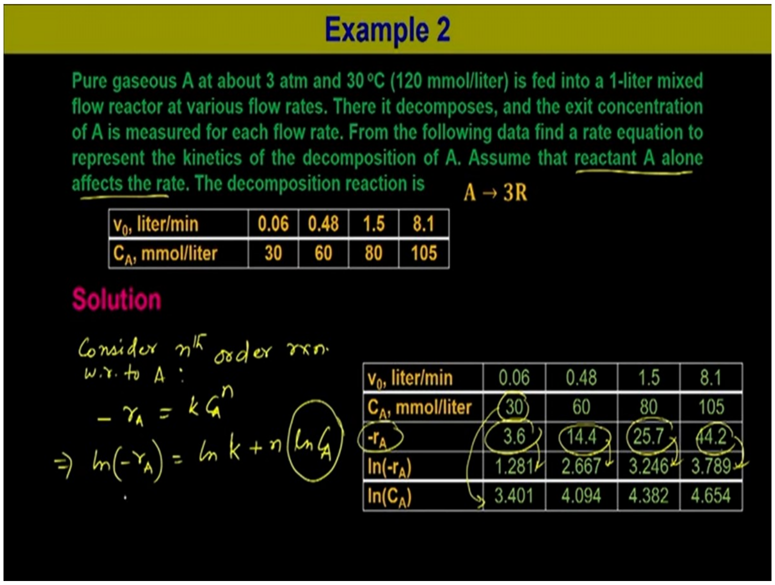

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v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105

Solution

Consider n^{th} order rxn. w.r.to A :

$$-r_A = kC_A^n$$

$$\Rightarrow \ln(-r_A) = \ln k + n\ln C_A$$

v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105
$-r_A$	3.6	14.4	25.7	44.2
$\ln(-r_A)$	1.281	2.667	3.246	3.789
$\ln(C_A)$	3.401	4.094	4.382	4.654

Now, if we consider nth order reaction with respect to A. Consider nth order reaction with respect to A. As it is said only reactant A alone affects the rate. So, we can write

$$-r_A = kC_A^n$$

Now, if we take log of these both sides it will be

$$\ln(-r_A) = \ln k + n\ln C_A$$

So now, we can calculate the data. So we have calculated different r_A values and we know the concentration so we can calculate the term $\ln(-r_A)$ so if we take from this data points so we can calculate ln terms, $\ln(-r_A)$. And since we know for each rate we know the concentration so we can calculate $\ln C_A$. So, in this equation we can calculate this part and we have calculated this part.

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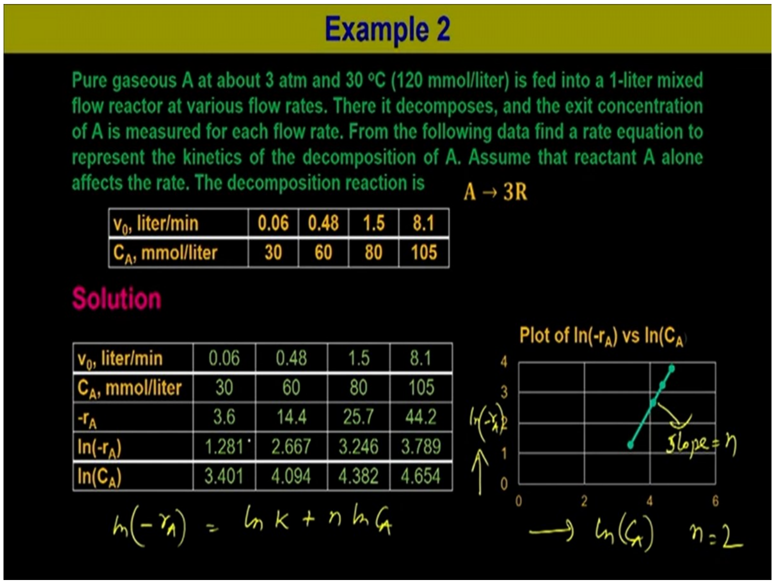

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Solution

v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105
$-r_A$	3.6	14.4	25.7	44.2
$\ln(-r_A)$	1.281	2.667	3.246	3.789
$\ln(C_A)$	3.401	4.094	4.382	4.654

Plot of $\ln(-r_A)$ vs $\ln(C_A)$

$\ln(-r_A) = \ln k + n \ln C_A$

$n = 2$

Now, if we plot these values $\ln(-r_A)$ versus $\ln C_A$ so, this is $\ln(-r_A)$ and this is $\ln C_A$. So this will give a straight line with a slope of that equation

$$\ln(-r_A) = \ln k + n \ln C_A$$

So, the slope of this curve is n. So, the slope can be calculated here the slope n = 2.

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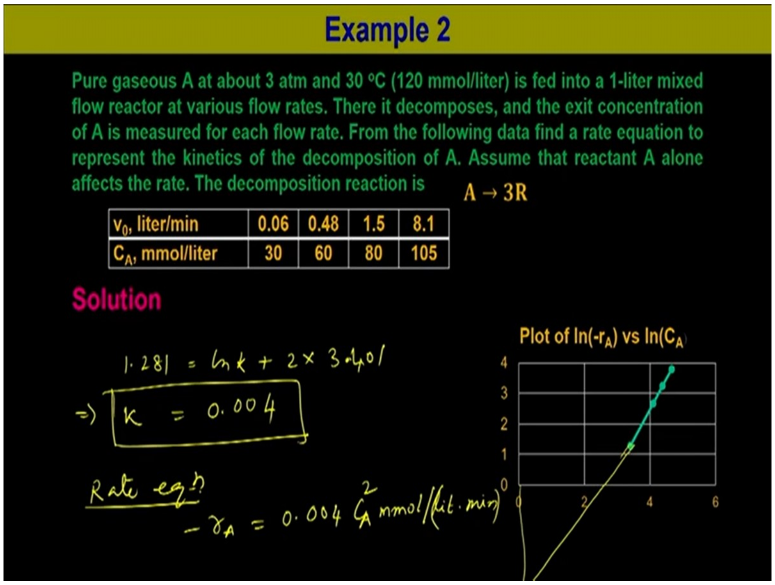

Example 2

Pure gaseous A at about 3 atm and 30 °C (120 mmol/liter) is fed into a 1-liter mixed flow reactor at various flow rates. There it decomposes, and the exit concentration of A is measured for each flow rate. From the following data find a rate equation to represent the kinetics of the decomposition of A. Assume that reactant A alone affects the rate. The decomposition reaction is $A \rightarrow 3R$

v_0, liter/min	0.06	0.48	1.5	8.1
C_A, mmol/liter	30	60	80	105

Solution

Plot of $\ln(-r_A)$ vs $\ln(C_A)$

$1.281 = \ln k + 2 \times 3.401$

$\Rightarrow \boxed{k = 0.004}$

Rate eqn

$-r_A = 0.004\, C_A^2$ mmol/(lit·min)

Now, we can either calculate the intercept which is ln k as per the equation or we can substitute in the any rate equation for any data points so we can write if we consider this first data point 1.281 and 3.401 so,

$$1.281 = \ln k + 2 * 3.401$$

if we put from here we can calculate k = 0.004.

So, once we calculate k or the same thing (calculate) extra plot this and we can calculate from the intercept. So the rate equation should be

$$-r_A = 0.004 C_A^2 mmol / (lit.\min)$$

So this way we can find out the rate equations for a particular reactor data. Thank you for attending this lecture and we will continue our discussion of reactor design in the next lecture and in the next lecture we will mostly consider design of the ideal plug flow reactor.