Chemical Reaction Engineering I
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Lecture 04
Introduction and Stoichiometry for the Batch System

Welcome to the first lecture of module 2 of Chemical Reaction Engineering 1. In this module we will discuss Stoichiometry. So before going to this lecture let us have brief recap on our previous lecture.

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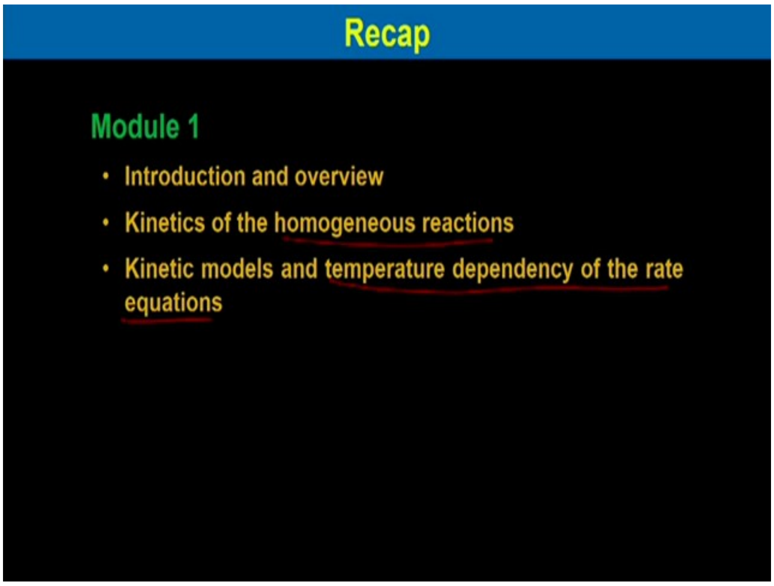

Recap

Module 1

- Introduction and overview
- Kinetics of the homogeneous reactions
- Kinetic models and temperature dependency of the rate equations

In our previous module which we had in the 3 lectures in our previous module. The first thing we have considered introduction and overview for the chemical reaction engineering course, then we have discussed the kinetics of the homogeneous reaction where we have considered different mechanisms which may occur and what is their kinetics of the reactions. The order of the reactions, the molecularity of the reactions and how to get the order of the reactions from a particular rate equations. Then we have classified the kinetics of the reactions into elementary and non-elementary reactions.

Then we have considered kinetic models that means rate equations and how to obtain rate equations from the different kinetic models. And how to test the models which we develop based on some particular mechanism that we have discussed in the last lecture. And we have also considered the temperature dependency of the rate equations that means the rate equations is related, is a function of temperature and the composition. The temperature dependency term is related to the rate coefficient and which is popularly well-known equations which is developed is the Arrhenius equation of the temperature dependency of the rate equations which we have considered and we have seen for a particular reaction, how to calculate the activation energy.

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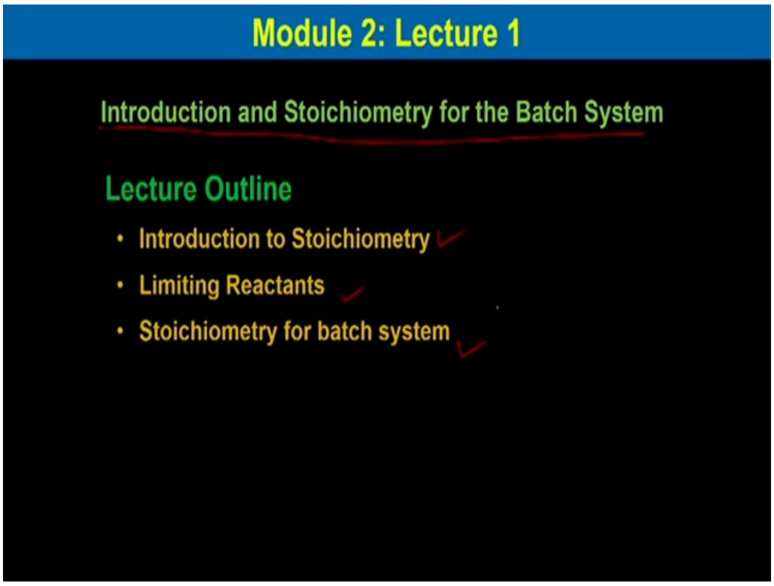

Module 2: Lecture 1

Introduction and Stoichiometry for the Batch System

Lecture Outline

- Introduction to Stoichiometry
- Limiting Reactants
- Stoichiometry for batch system

Now in this lecture, we will consider introduction to Stoichiometry, introduction and Stoichiometry of the batch reactor systems. So the brief lecture outline would be introduction to Stoichiometry, why it is important? And what are the things we need to take care while designing the reactor, then limiting reactants and then we will consider Stoichiometry for the batch system.

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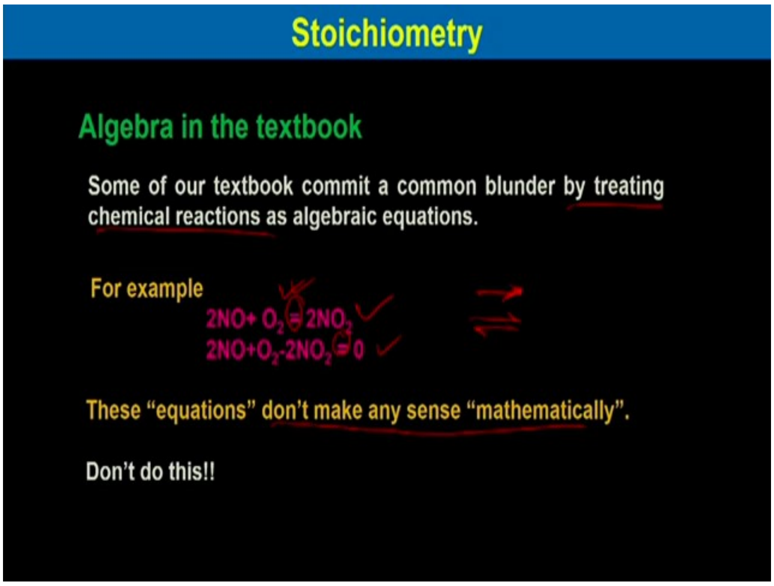

Stoichiometry

Algebra in the textbook

Some of our textbook commit a common blunder by treating chemical reactions as algebraic equations.

For example

$$2NO + O_2 = 2NO_2$$

$$2NO + O_2 - 2NO_2 = 0$$

These "equations" don't make any sense "mathematically".

Don't do this!!

In most of or some of our algebra in the textbook is commit some common mistakes by treating chemical reactions as algebraic equations. That means

For example if we consider nitric oxide reacts with oxygen and form nitrogen dioxide and it is written like this.

$$2NO + O_2 = 2NO_2$$

And then we can just take the twice NO2 on the left side we can write twice NO plus oxygen minus twice NO2 is equal to 0.

$$2NO + O_2 - 2NO_2 = 0$$

Whether this equation or this chemical reactions are correct? These 2 reactions, whether they are correct? Or representation are correct? As you can see these are represented with the equality sign. So chemical reaction cannot be represented with the equality sign. So this is nOT correct. So in some of the textbook you will notice like this. This equation don’t make any sense mathematically. So don’t do this.

So while writing chemical reactions we must be careful that whether the reaction is irreversible in nature or reversible in nature. So based on that we have to include this sign. So we cannot use like a mathematics. So like we have to write either know this arrow forward or we can write the reversible sign. So for chemical reactions this has to be represented at with a particular notations. So while doing your chemical reaction engineering derivations of the rate equations and so on or the mechanism of the reactions we must be very careful about writing the chemical reaction.

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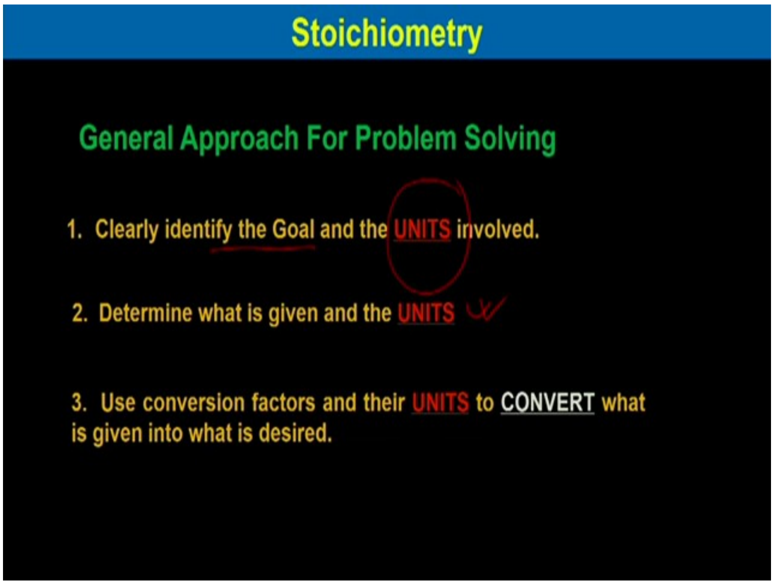

Stoichiometry

General Approach For Problem Solving

1. Clearly identify the Goal and the UNITS involved.
2. Determine what is given and the UNITS
3. Use conversion factors and their UNITS to CONVERT what is given into what is desired.

The general approach to the Stoichiometry is that for solving any problem we must be very cautious about the units of the different concentration or different terms given for the particular problem. So we should follow a general guidelines. One is clearly identify the goal what you need to do and then what are the units involved in that particular goal then the second thing is that determined what is given and the units.

The second step you need to follow is what is given and what are their units. And then the third thing use the conversion factor, their units to convert what is given into what is desired. So this conversion of the conversion factor has to be based on the particular units. So we must be careful while solving some particular problem in case of Stoichiometry or any other problem when we are going to solve it.

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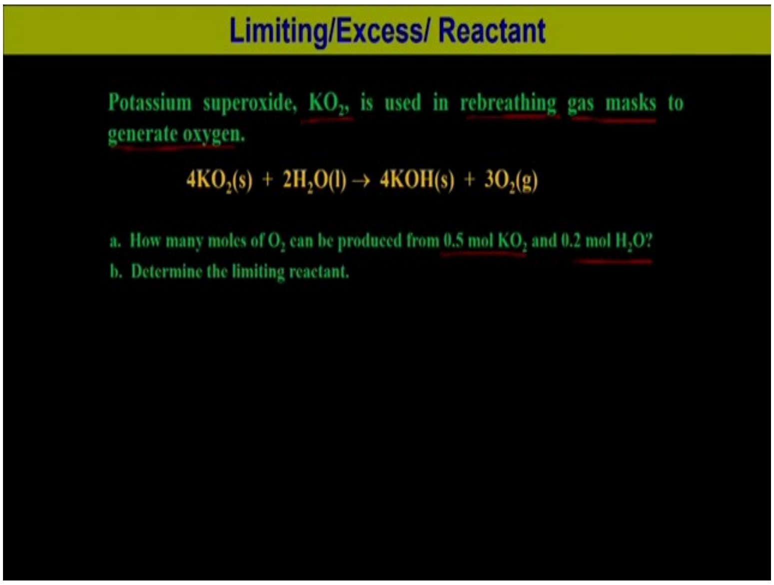

Limiting/Excess/ Reactant

Potassium superoxide, KO_2, is used in rebreathing gas masks to generate oxygen.

$$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$$

a. How many moles of O_2 can be produced from 0.5 mol KO_2 and 0.2 mol H_2O?
b. Determine the limiting reactant.

While solving reactions we must know what is the limiting reactants for a particular reactions? Like if we consider potassium superoxide KO_2 is used for rebreathing gas mask to generate oxygen.

The reactions,

$$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$$

So this KO_2 potassium superoxide or potassium dioxide it forms oxygen, so its mask is used as an oxygen generator.

Now, the problem is how many moles of oxygen can be produced from 0.5 mole of KO_2 to and 0.2 mole of H_2O. So the given for these reactants 0.5 mole KO_2 and 0.2 mole of H_2O. And we have to find out which one is the limiting reactants because the initial concentration for both the reactants are given.

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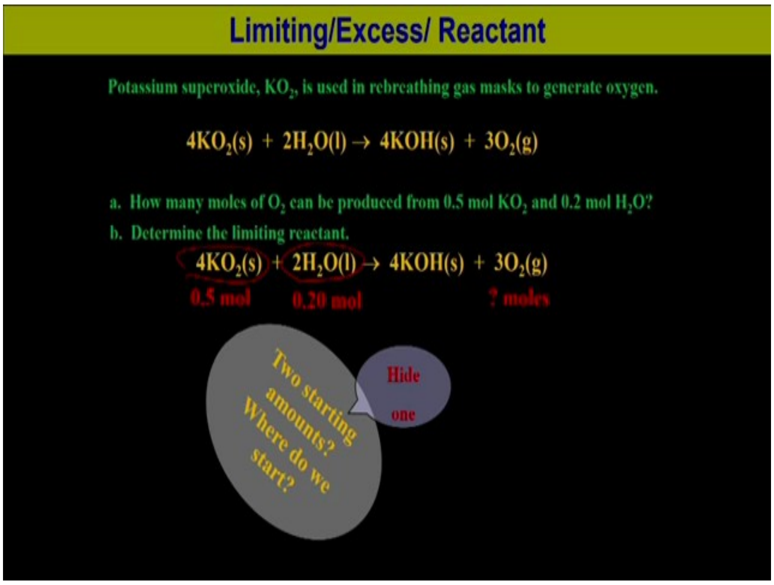

Limiting/Excess/ Reactant

Potassium superoxide, KO_2, is used in rebreathing gas masks to generate oxygen.

$$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$$

a. How many moles of O_2 can be produced from 0.5 mol KO_2 and 0.2 mol H_2O?
b. Determine the limiting reactant.

$$\underset{0.5\ \text{mol}}{4KO_2(s)} + \underset{0.20\ \text{mol}}{2H_2O(l)} \rightarrow 4KOH(s) + \underset{?\ \text{moles}}{3O_2(g)}$$

So this is the reaction and these are given 0.5 mole of KO_2 and 0.2 mole of H_2O and we have to find out the moles of oxygen produced. So we have 2 starting materials, one is KO_2 and another one is H_2O and we have to choose any one first.

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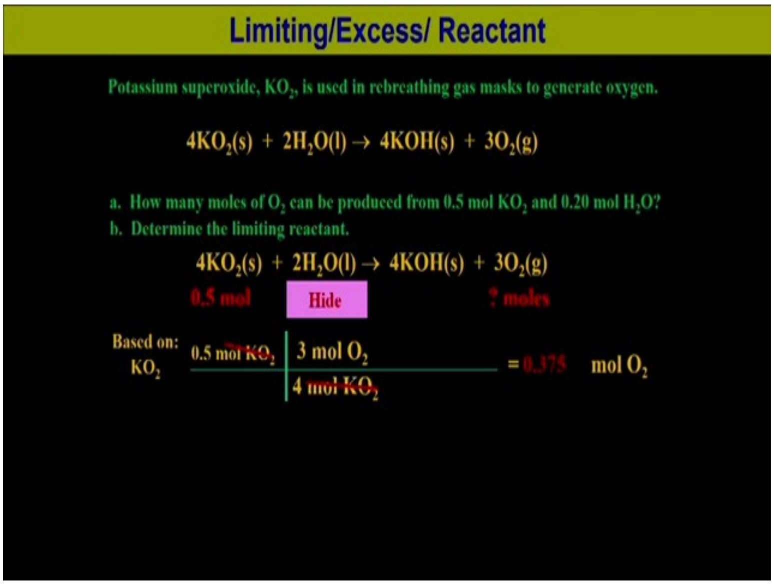

Limiting/Excess/ Reactant

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$$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$$

a. How many moles of O_2 can be produced from 0.5 mol KO_2 and 0.20 mol H_2O?
b. Determine the limiting reactant.

$$\underset{0.5\ \text{mol}}{4KO_2(s)} + \underset{\text{Hide}}{2H_2O(l)} \rightarrow 4KOH(s) + \underset{?\ \text{moles}}{3O_2(g)}$$

Based on: KO_2

$$\frac{0.5\ \cancel{\text{mol } KO_2}}{} \left| \frac{3\ \text{mol } O_2}{4\ \cancel{\text{mol } KO_2}} \right. = 0.375\ \text{mol } O_2$$

So let us hide water, so if we consider based on KO_2 as a basis of the reactants then we need to obtain the mole of oxygen produced if KO_2 is the basis of the reaction. Now, how much is given KO_2 is 0.5 mole of KO_2 and then as per the Stoichiometry of the reactions 4 mole of KO_2 reacts with 2 mole of water produced 3 mole of oxygen. So our moles of oxygen produced is 3 mole as per the Stoichiometry and that produced from 4 mole of KO_2. So if we write these two, then this 4 mole KO_2 and 0.5 mole KO_2 will cancel out, okay. And then we can calculate the mole of oxygen produced that is 0.375 mole of oxygen.

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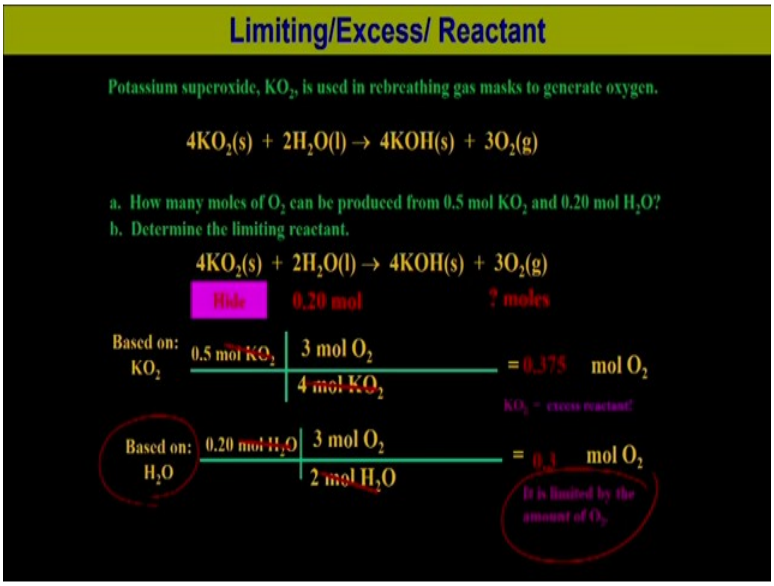

Limiting/Excess/ Reactant

Potassium superoxide, KO_2, is used in rebreathing gas masks to generate oxygen.

$$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$$

a. How many moles of O_2 can be produced from 0.5 mol KO_2 and 0.20 mol H_2O?

b. Determine the limiting reactant.

$$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$$

Hide 0.20 mol ? moles

Based on: KO_2

$$0.5\ \cancel{\text{mol } KO_2} \times \frac{3 \text{ mol } O_2}{4\ \cancel{\text{mol } KO_2}} = 0.375 \text{ mol } O_2$$

KO_2 = excess reactant!

Based on: H_2O

$$0.20\ \cancel{\text{mol } H_2O} \times \frac{3 \text{ mol } O_2}{2\ \cancel{\text{mol } H_2O}} = 0.3 \text{ mol } O_2$$

It is limited by the amount of O_2

Now, if we consider the water as the basis instead of KO_2. Let us hide KO_2 and consider water as the basis. So, if we consider basis as water then we can see that 0.2 mole of water is given initially and then as per the Stoichiometry 2 mole of water forms 3 moles of oxygen.

So produced 3 mole of oxygen from 2 mole of water. So this mole water and mole water they will cancel out and you will obtain 0.3 mole of oxygen, so as we can see from this mole valance we can see that the minimum oxygen produced from these 2 reactants is based on the water that is 0.3 mole of oxygen. That means this water is the limiting reactants, and so the limiting reactants is water over here for the production of oxygen because this is the minimum quantity produced compared to based on KO_2. And KO_2 is the excess reactant. So this way we can find out what is the limiting reactants.

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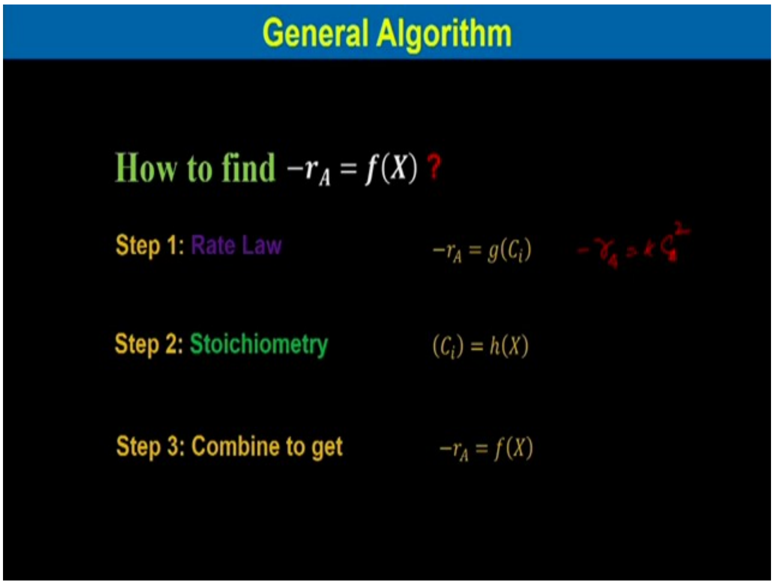

General Algorithm

How to find $-r_A = f(X)$?

Step 1: Rate Law $-r_A = g(C_i)$ $-r_A = kC_A^2$

Step 2: Stoichiometry $(C_i) = h(X)$

Step 3: Combine to get $-r_A = f(X)$

So our general algorithm for any Stoichiometry related problem would be, the idea is to how to find out the rate of reactions as a function of conversion. In a particular reactant which will reacts and convert to products. The conversion, the extent of reactions or the conversion factor can be how to relate with the rate of reaction. So the step to be followed, in the first step we should know the rate law.

Like,

Step 1: $$-r_A = g(C_i)$$

$-r_A$ is a function of concentration, as we have said earlier minus if it is second-order reactions it would be say

$$-r_A = kC_A^2$$

So it is a concentration dependent term, so this is the rate law. The second step would be the Stoichiometry, how the concentration is related to conversion.

Step 2: $$(C_i) = h(X)$$

So concentration is a function of conversion and third step would be combined these two to get

Step 3: $$-r_A = f(X)$$

So these are the general procedure we need to follow.

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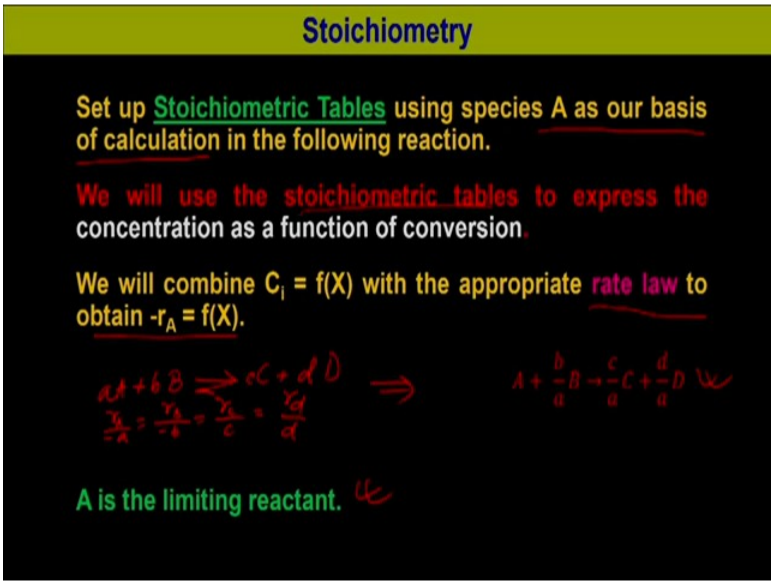

Stoichiometry

Set up Stoichiometric Tables using species A as our basis of calculation in the following reaction.

We will use the stoichiometric tables to express the concentration as a function of conversion.

We will combine $C_i = f(X)$ with the appropriate rate law to obtain $-r_A = f(X)$.

$aA + bB \rightarrow cC + dD$ $\Rightarrow$ $A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$

$\frac{r_A}{-a} = \frac{r_B}{-b} = \frac{r_C}{c} = \frac{r_D}{d}$

A is the limiting reactant.

Now, we need to set up a stoichiometric table using spaces A as a basis of calculation in the following reactions. So to find out the relation between rate of reactions with the conversion we need to make a stoichiometric tables. Stoichiometric table is nothing but, it is a balanced table for the conversion of reactants to products for a single reaction.

So suppose there is a reaction

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

From this as we have earlier said this would be

$$-\frac{r_A}{A} = -\frac{r_B}{B} = \frac{r_C}{C} = \frac{r_D}{D}$$

So from here we can write if A is our basis of the calculation so this reaction we can write,

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

So this is written with per mole of A. This reaction is written per mole of A. Now, we will use the stoichiometric table to express the concentration as a function of conversion. And then we need to combine concentration as a function of X that is the conversion with appropriate rate law to obtain $-r_A$ as a function of X. So A is over here is the limiting reactant as I have said already.

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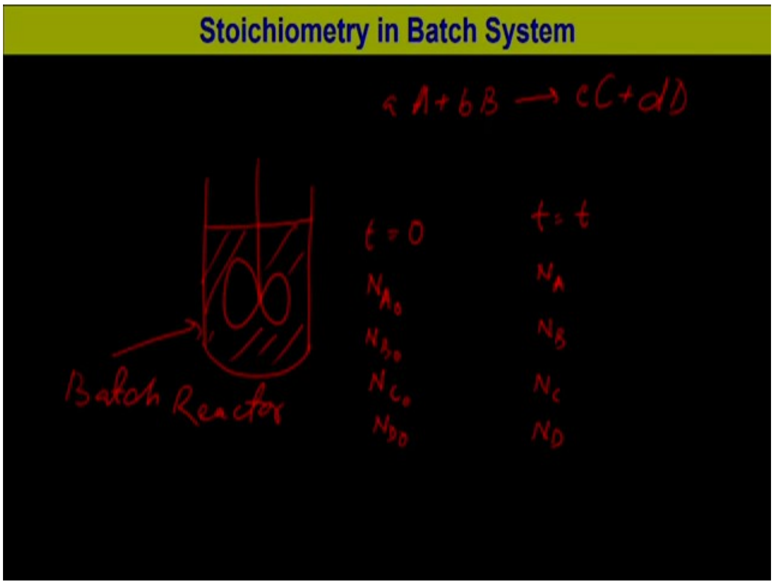

Stoichiometry in Batch System

So now, let us consider a batch system, so this is the batch reactor and where you have the content, all the content over here initially and it is closed. At t is equal to zero, your condition is you have reactant NA naught, so the reaction is

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

So this at t is equal to zero the initial moles of all the reactants and products are given that is $N_{A0}, N_{B0}, N_{C0}, N_{D0}$.

At t is equal to t this is N_A the concentration of A is N_A, concentration of B is N_B, concentration of C is N_C and concentration of D is N_D, so this is batch reactor. Now we have to do the mole balance which is reacting over here, so how much the reactants initially presents and how much A is reacting with B and how much product is produced.

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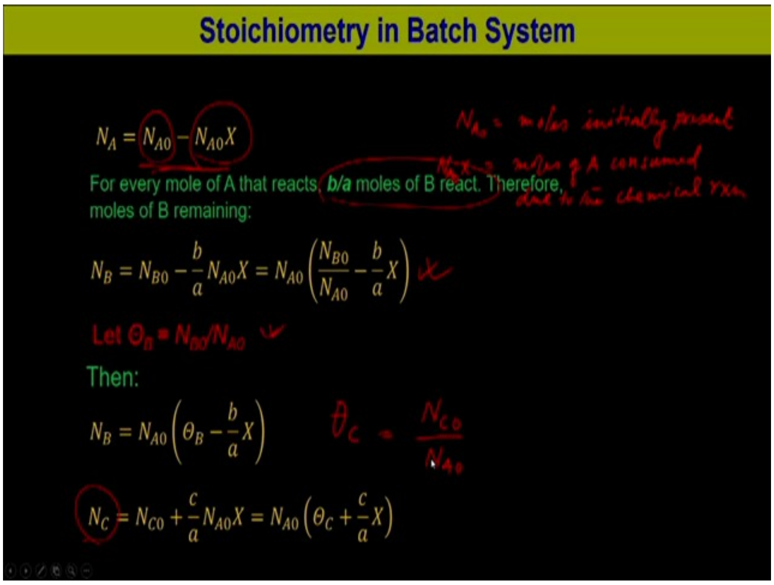

Stoichiometry in Batch System

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

For every mole of A that reacts, *b/a* moles of B react. Therefore, moles of B remaining:

$N_B = N_{B0} - \frac{b}{a}N_{A0}X = N_{A0}\left(\frac{N_{B0}}{N_{A0}} - \frac{b}{a}X\right)$ ✓

Let $\Theta_B = N_{B0}/N_{A0}$ ✓

Then:

$N_B = N_{A0}\left(\Theta_B - \frac{b}{a}X\right)$ $\theta_C = \frac{N_{C0}}{N_{A0}}$

$N_C = N_{C0} + \frac{c}{a}N_{A0}X = N_{A0}\left(\Theta_C + \frac{c}{a}X\right)$

N_{A0} = moles initially present

$N_{A0}X$ = moles of A consumed due to the chemical rxn

So to do that, if we consider initially for the reactions we had N_A moles of A N_{A0} that is the initial concentration and from the Stoichiometry as we can see that one mole of A is reacting and producing C and D, so the conversion factor X, so N_{A0} X is consumed, reactant which is consumed, So the remaining amount is,

$$N_{A0} - N_{A0}X$$

So

N_{A0} = moles initially present,

$N_{A0}X$ = moles of A consumed due to the chemical reactions.

So we will have

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

Now, for every mole of A that reacts $\frac{b}{a}$ moles of B reacts. Therefore, the moles of B would be remaining as

$$N_B = N_{B0} - \frac{b}{a}N_{A0}X = N_{A0}\left(\frac{N_{B0}}{N_{A0}} - \frac{b}{a}X\right)$$

Let

$$\Theta_B = \frac{N_{B0}}{N_{A0}}$$

Θ_B is the ratio of initial mole of B divided by initial mole of A. So this is Θ_B. Then we can write

$$N_B = N_{A0}(\Theta_B - \frac{b}{a}X)$$

So since NB naught by NA naught is the ratio of the moles, so it is dimension less term, so theta b which is further simplification we can write this way. Similarly, we can write

$$N_C = N_{C0} + \frac{c}{a}N_{A0}X$$

This N_C is the product which is produced and how much moles of N_C is produced is

$$\frac{c}{a}N_{A0}X$$

This is based on the Stoichiometry of the chemical reaction.

And similar way if we define Θ_C which is

$$\Theta_C = \frac{N_{C0}}{N_{A0}}$$

So it would be

$$N_{A0}(\Theta_C - \frac{c}{a}X)$$

So here

$$\Theta_C = \frac{N_{C0}}{N_{A0}}$$

Similarly, we can write for the product D.

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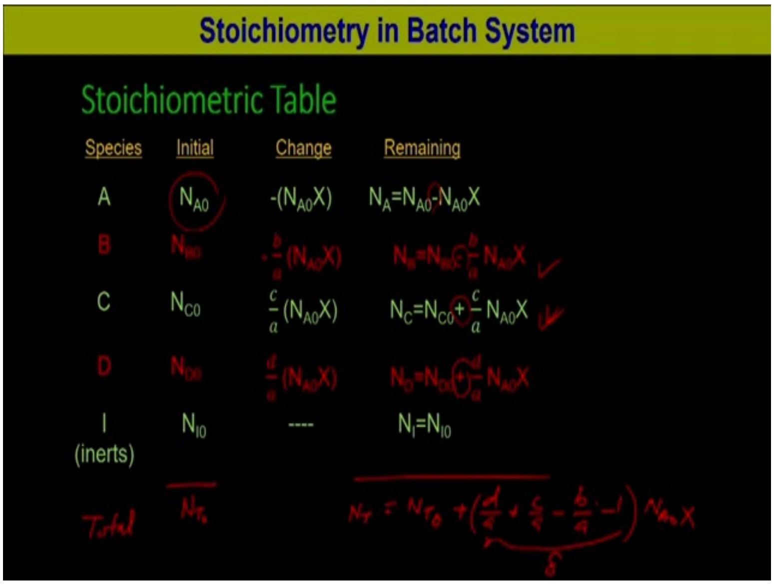

Stoichiometry in Batch System

Stoichiometric Table

Species	Initial	Change	Remaining
A	N_{A0}	$-(N_{A0}X)$	$N_A=N_{A0}-N_{A0}X$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X)$	$N_B=N_{B0}-\frac{b}{a}N_{A0}X$ ✓
C	N_{C0}	$\frac{c}{a}(N_{A0}X)$	$N_C=N_{C0}+\frac{c}{a}N_{A0}X$ ✓
D	N_{D0}	$\frac{d}{a}(N_{A0}X)$	$N_D=N_{D0}+\frac{d}{a}N_{A0}X$
I (inerts)	N_{I0}	----	$N_I=N_{I0}$
Total	N_{T_0}		$N_T = N_{T_0} + \underbrace{\left(\frac{d}{a}+\frac{c}{a}-\frac{b}{a}-1\right)}_{\delta} N_{A0}X$

Now, we need to develop the stoichiometric table. So in the stoichiometric table let us write species, initial, change of concentration and what is the remaining concentration. So initially we have this is A which is concentration initially N_{A0} and its change due to the chemical reaction is $-N_{A0}X$ and then the amount remaining N_A which is $N_A = N_{A0} - N_{A0}X$.

For species B initial concentration is N_{B0}, then the change of concentration due to the chemical reaction this mass is reacted that is $-\frac{b}{a}N_{A0}X$, so N_B would be $N_{B0} - \frac{b}{a}N_{A0}X$. Now for the product C, initial concentration was N_{C0} and the product which is produced due to the chemical reaction is $\frac{c}{a}N_{A0}X$. So N_C would be $N_C = N_{C0} + \frac{c}{a}N_{A0}X$ that is a product which is after A time of t.

Similarly, for D we can write, N_{D0} is the initial concentration $\frac{d}{a}N_{A0}X$ and the remaining one would be $N_{D0} + \frac{d}{a}N_{A0}X$. So for the product it is increasing from the initial concentration, for the reactants these are decreasing after the chemical reactions, so that is why from the initial this is represented with the negative sign and this is represented with the positive sign.

Now for the reaction to happen if we have some inert gas or inert reactant present initially, so we need to also consider what would happen to that inert? So initially suppose I is the inert and its initial concentration is N_{I0}. So because it is inert and not taking part into the chemical reaction, so it will not change its concentration. So whatever initially present of that inert will remain that is N_I would be N_{I0}.

Now, if we make the total, so this would be N_{T0} and which we can just add them, all of them

$$N_{A0} + N_{B0} + N_{C0} + N_{D0} + N_{I0}$$

These are the initial concentration N_T and then we can obtain the N_T from here which is remaining, so we can write

$$N_T = N_{T0} + (\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1)N_{A0}X$$

So this is the δ.

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

So this can be called as δ. This coefficient is δ. So this way we can develop the stoichiometric table.

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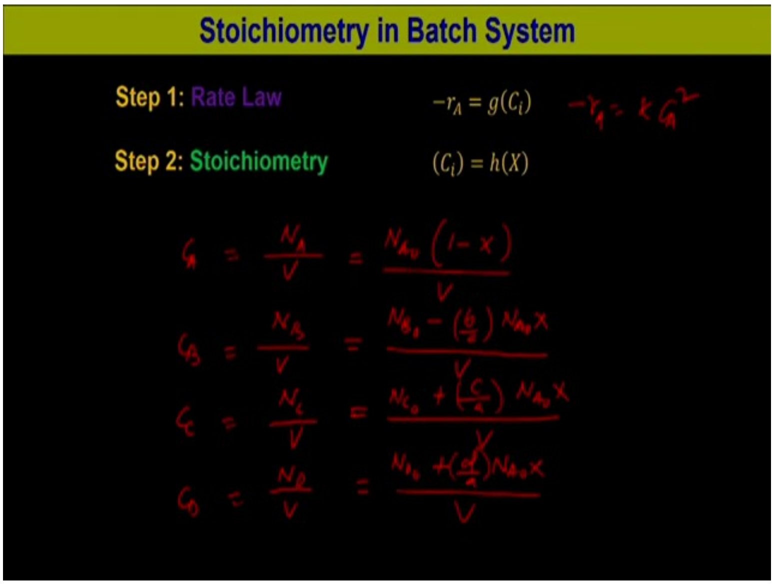

Stoichiometry in Batch System

Step 1: Rate Law $-r_A = g(C_i)$ $-r_A = kC_A^2$

Step 2: Stoichiometry $(C_i) = h(X)$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V}$$

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - \left(\frac{b}{a}\right)N_{A0}X}{V}$$

$$C_C = \frac{N_C}{V} = \frac{N_{C0} + \left(\frac{c}{a}\right)N_{A0}X}{V}$$

$$C_D = \frac{N_D}{V} = \frac{N_{D0} + \left(\frac{d}{a}\right)N_{A0}X}{V}$$

Now, our step one is

Step 1: $$-r_A = g(C_i)$$

$-r_A$, the rate of reaction is a function of concentration and Step 2 is the concentration should be relations between concentrations with the conversion.

Step 2: $$(C_i) = h(X)$$

Now if we consider concentration of A is the moles per unit volume if we can write, so for this a

$$-r_A = kC_A^2$$

Now we need to convert concentration to conversion, first we know the moles which is reacting, so we need to write moles in terms of the concentration.

So if we divide with the volume of the reactants, so it will give the concentration. So write concentration of A would be

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

So this is per unit volume. So then we can write

$$C_A = \frac{N_{A0}(1-X)}{V}$$

Similarly we can write

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - (\frac{b}{a})N_{A0}X}{V}$$

In case of product that is

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

For D that is

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

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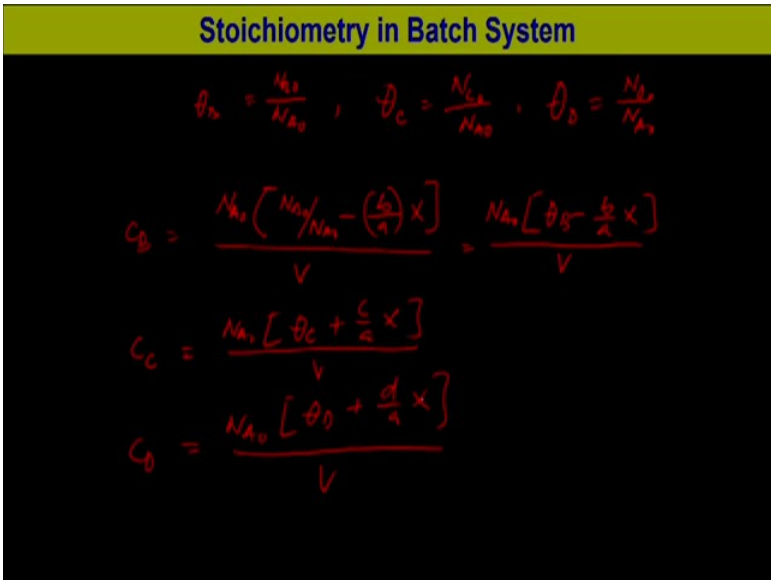

Stoichiometry in Batch System

$$\theta_B = \frac{N_{B0}}{N_{A0}}, \quad \theta_C = \frac{N_{C0}}{N_{A0}}, \quad \theta_D = \frac{N_{D0}}{N_{A0}}$$

$$C_B = \frac{N_{A0}\left(N_{B0}/N_{A0} - \left(\frac{b}{a}\right)X\right]}{V} = \frac{N_{A0}\left[\theta_B - \frac{b}{a}X\right]}{V}$$

$$C_C = \frac{N_{A0}\left[\theta_C + \frac{c}{a}X\right]}{V}$$

$$C_D = \frac{N_{A0}\left[\theta_D + \frac{d}{a}X\right]}{V}$$

Now, if we further simplifying this term by defining Θ_B as $\frac{N_{B0}}{N_{A0}}$, Θ_C is $\frac{N_{C0}}{N_{A0}}$ and Θ_D is $\frac{N_{D0}}{N_{A0}}$, so if we define these theta term then we can write

$$C_B = \frac{N_{A0}[\frac{N_{B0}}{N_{A0}} - (\frac{b}{a})X]}{V}$$

So this would be

$$C_B = \frac{N_{A0}[\Theta_B - (\frac{b}{a})X]}{V}$$

Similarly, we can write

$$C_C = \frac{N_{A0}[\Theta_C - (\frac{c}{a})X]}{V}$$

and

$$C_D = \frac{N_{A0}[\Theta_D - (\frac{d}{a})X]}{V}$$

So this way we can write the concentration terms in terms of the conversion X.

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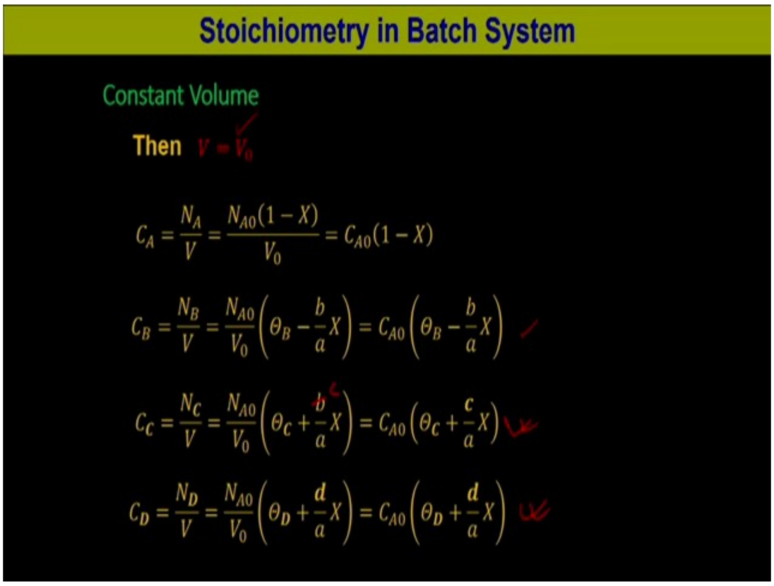

Stoichiometry in Batch System

Constant Volume

Then $V = V_0$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V_0} = C_{A0}(1-X)$$

$$C_B = \frac{N_B}{V} = \frac{N_{A0}}{V_0}\left(\theta_B - \frac{b}{a}X\right) = C_{A0}\left(\theta_B - \frac{b}{a}X\right)$$

$$C_C = \frac{N_C}{V} = \frac{N_{A0}}{V_0}\left(\theta_C + \frac{b}{a}X\right) = C_{A0}\left(\theta_C + \frac{c}{a}X\right)$$

$$C_D = \frac{N_D}{V} = \frac{N_{A0}}{V_0}\left(\theta_D + \frac{d}{a}X\right) = C_{A0}\left(\theta_D + \frac{d}{a}X\right)$$

Now, if we consider constant volume batch reactor system then our V could be

$$V = V_0$$

Which is the initial volume there is no change of the volume of the reactants or the system. So we can then write

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

So V we can substitute with V_0, so $\frac{N_{A0}}{V_0}$ which is constant can write

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

Similarly we can write for C_B

$$C_B = \frac{N_B}{V} = \frac{N_{A0}}{V_0}(\Theta_B - (\frac{b}{a})X)$$

So which would be

$$C_B = C_{A0}(\Theta_B - (\frac{b}{a})X)$$

And for C_C we can write

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

So this would be

$$C_C = C_{A0}(\Theta_c + (\frac{c}{a})X)$$

So this is for C_C.

Now, for C_D also similar way we can write

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

which is equal to

$$C_D = C_{A0}(\Theta_D + (\frac{d}{a})X)$$

So for constant volume batch reactor we can write the concentration term with the conversion and the initial concentration of the reactant A.

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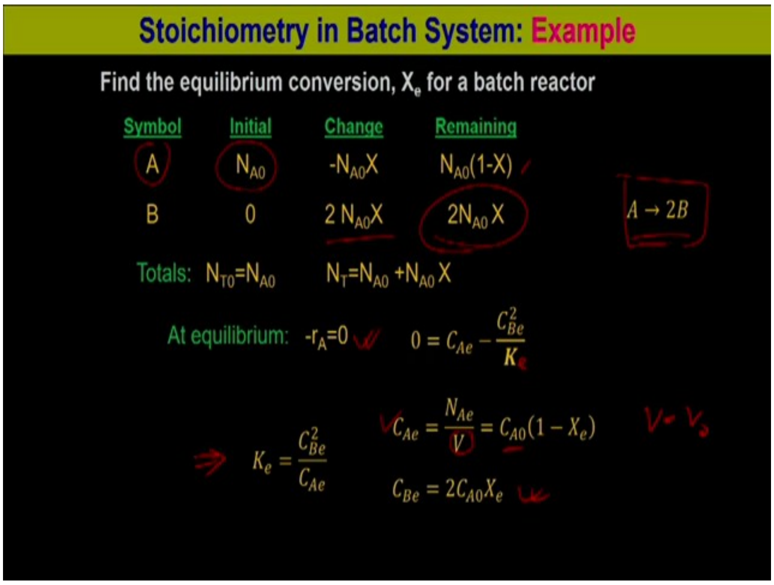

Stoichiometry in Batch System: Example

Find the equilibrium conversion, X_e for a batch reactor

Symbol	Initial	Change	Remaining
A	N_{A0}	$-N_{A0}X$	$N_{A0}(1-X)$
B	0	$2\,N_{A0}X$	$2N_{A0}X$

$A \rightarrow 2B$

Totals: $N_{T0}=N_{A0}$ $N_T=N_{A0}+N_{A0}X$

At equilibrium: $-r_A=0$ $0 = C_{Ae} - \frac{C_{Be}^2}{K_e}$

$$C_{Ae} = \frac{N_{Ae}}{V} = C_{A0}(1-X_e)$$

$V = V_0$

$$\Rightarrow K_e = \frac{C_{Be}^2}{C_{Ae}}$$

$$C_{Be} = 2C_{A0}X_e$$

Now, let us consider an example for the batch system. Consider the following elementary reactions with equilibrium constant K = 50 litre per mole and initial reactant concentration C_{A0} is 0.5 mole per litre. The reactions

$$A \rightleftharpoons B$$

and the rate of reactions is given as

$$-r_A = k_A[C_A - \frac{C_B^2}{K}]$$

K is the equilibrium constant.

We need to find out the equilibrium conversion X_e for the batch reactor.

Now, our objective is to calculate X_e, we need to see what are given, so K is given that is 50 litre per mole and the initial concentration C_{A0} is given which is 0.5 mole per litre. Now, we need to follow the steps. First step we should know the relations

Step 1: $$\frac{dX}{dt} = \frac{-r_A V}{N_{A0}}$$

that is the rate law and the rate law which is given over here is, so that is $-r_A$ has to be related with the concentration that is

Step 2: Rate Law $$-r_A = k_A C_A - k_B C_B^2$$

And then from here you can write

$$-r_A = k_A[C_A - \frac{C_B^2}{K}]$$

so this K is nothing but

$$K = \frac{k_A}{k_B}$$

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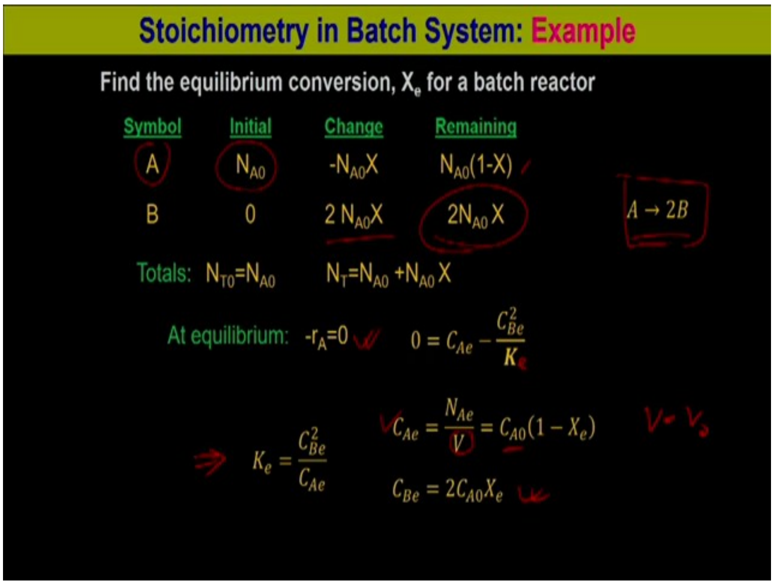

Stoichiometry in Batch System: Example

Find the equilibrium conversion, X_e for a batch reactor

Symbol	Initial	Change	Remaining
A	N_{A0}	$-N_{A0}X$	$N_{A0}(1-X)$
B	0	$2N_{A0}X$	$2N_{A0}X$

$A \rightarrow 2B$

Totals: $N_{T0}=N_{A0}$ $\quad N_T=N_{A0}+N_{A0}X$

At equilibrium: $-r_A=0$ $\quad 0 = C_{Ae} - \frac{C_{Be}^2}{K_e}$

$$C_{Ae} = \frac{N_{Ae}}{V} = C_{A0}(1-X_e) \qquad V = V_0$$

$$\Rightarrow K_e = \frac{C_{Be}^2}{C_{Ae}} \qquad C_{Be} = 2C_{A0}X_e$$

Now, we need to find the conversion X_e for a batch reactor and this is the reaction. So we need to obtain the Stoichiometry table for the relations, so N_A, so A reactants is converting its initial concentration N_{A0} and change would be $N_{A0}X$ and remaining would be $N_{A0}(1-X)$. X is the conversion, now for component B if we look into this reaction Stoichiometry that 2 moles of B is produced, so initially B was zero.

So only the A is present initially, there is no B into the system, so initial B is zero and change would be $2N_{A0}X$ and then the remaining would be $2N_{A0}X$ for B which is the product. Now the total N_{T0} would be

$$N_{T0} = N_{A0}$$

Here initial and N_T would be if you just add them that is

$$N_T = N_{A0} + N_{A0}X$$

At equilibrium,

$$-r_A = 0$$

As you know, so if we write from the rate equation, so this would be zero.

At equilibrium can write that concentration is C_{Ae} that is the equilibrium concentration and for B it is C_{Be}. So this would be $\frac{C_{Be}^2}{K_e}$. So from here we can write K_e

So this is nothing but K_e, so from this relations at equilibrium if we apply $-r_A$ would be zero at equilibrium then we can write this relation as this. The rate equations we can write like this.

And from here we can write Ke would be

$$K_e = \frac{C_{Be}^2}{C_{Ae}}$$

C_{Ae} is nothing but

$$C_{Ae} = \frac{N_{Ae}}{V}$$

As V is for the constant volume system V is V_0, so

$$\frac{N_{Ae}}{V_0} = C_{A0}(1 - X_e)$$

So

$$C_{Ae} = C_{A0}(1 - X_e)$$

And CBe would be

$$C_{Be} = 2C_{A0}X_e$$

So now we obtained C_{Ae} the equilibrium conversion in terms of X_e and the equilibrium concentration in terms of X_e and then equilibrium concentration of B in terms of X_e.

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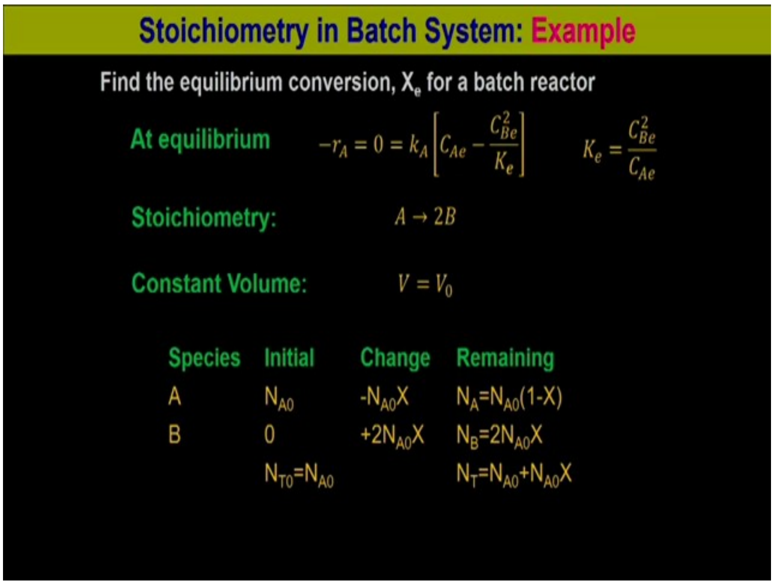

Stoichiometry in Batch System: Example

Find the equilibrium conversion, X_e for a batch reactor

At equilibrium $-r_A = 0 = k_A\left[C_{Ae} - \frac{C_{Be}^2}{K_e}\right]$ $K_e = \frac{C_{Be}^2}{C_{Ae}}$

Stoichiometry: $A \rightarrow 2B$

Constant Volume: $V = V_0$

Species	Initial	Change	Remaining
A	N_{A0}	$-N_{A0}X$	$N_A=N_{A0}(1-X)$
B	0	$+2N_{A0}X$	$N_B=2N_{A0}X$
	$N_{T0}=N_{A0}$		$N_T=N_{A0}+N_{A0}X$

Now at equilibrium, so this is the relation

$$-r_A = 0 = k_A[C_{Ae} - \frac{C_{Be}^2}{K_e}]$$

and

$$K_e = \frac{C_{Be}^2}{C_{Ae}}$$

From Stoichiometry we have

$$A \rightarrow 2B$$

And the volume is constant V is equal to V_0 and then this is our stoichiometric table, so this is the overall process which we have done so far. Equilibrium, Stoichiometry, constant volume and then we have obtained this.

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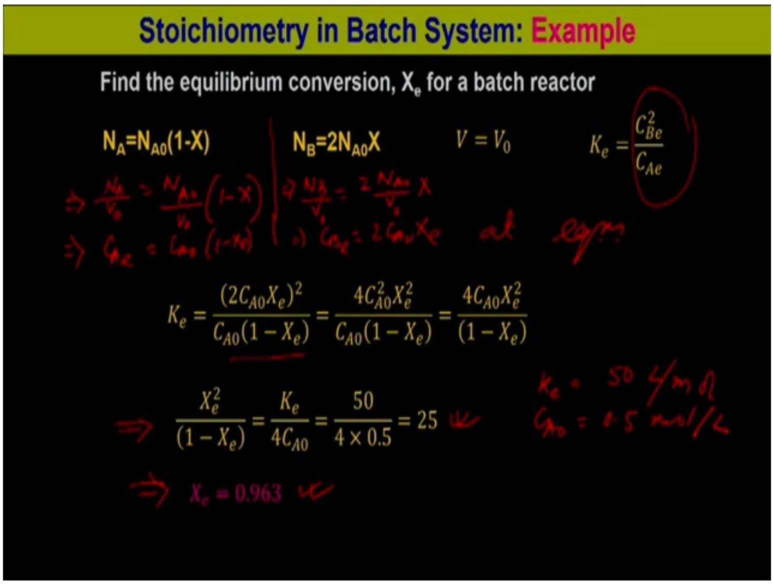

Stoichiometry in Batch System: Example

Find the equilibrium conversion, X_e for a batch reactor

$N_A=N_{A0}(1-X)$ | $N_B=2N_{A0}X$ | $V = V_0$ | $K_e = \frac{C_{Be}^2}{C_{Ae}}$

$\Rightarrow \frac{N_A}{V_0} = \frac{N_{A0}}{V_0}(1-X)$ | $\Rightarrow \frac{N_B}{V_0} = 2\frac{N_{A0}}{V_0}X$

$\Rightarrow C_{Ae} = C_{A0}(1-X_e)$ | $\Rightarrow C_{Be} = 2C_{A0}X_e$ at eqm

$$K_e = \frac{(2C_{A0}X_e)^2}{C_{A0}(1-X_e)} = \frac{4C_{A0}^2X_e^2}{C_{A0}(1-X_e)} = \frac{4C_{A0}X_e^2}{(1-X_e)}$$

$K_e = 50$ l/mol

$C_{A0} = 0.5$ mol/L

$$\Rightarrow \frac{X_e^2}{(1-X_e)} = \frac{K_e}{4C_{A0}} = \frac{50}{4\times 0.5} = 25$$

$$\Rightarrow X_e = 0.963$$

Now, N_A is $N_{A0}(1-X)$. N_B would be $2N_{A0}X$ and V is V_0 and K_e is $\frac{C_{Be}^2}{C_{Ae}}$. So if we just divide with V_0, $\frac{N_B}{V_0}$ would be $\frac{2N_{A0}X}{V_0}$. So this is nothing but C_A would be $C_{A0}(1-X)$ and from here C_{Be} would be $2C_{A0}X_e$. So now, if we substitute these C_{Ae} and C_{Be} we would obtain at equilibrium this would be X_e and this would be X_e and this is C_{Be} and this is C_{Ae} that is at equilibrium.

So, if we substitute these two over here, so we would obtain, this is

$$K_e = \frac{(2C_{A0}X_e)^2}{C_{A0}(1-X_e)}$$

which is written over here. So if we simplify this would be

$$K_e = \frac{4C_{A0}X_e^2}{(1-X_e)}$$

Now, if we just rearrange this relation we will get

$$\frac{X_e^2}{(1-X_e)} = \frac{K_e}{4C_{A0}}$$

Now, K_e is given 50 litre per mole and C_{A0} is given 0.5 mole per litre. So, if we substitute over here this would be

$$\frac{K_e}{4C_{A0}} = \frac{50}{4*0.5} = 25$$

Now, if we solve it for X_e, so you will get both positive and negative roots, but the convergence cannot be negative. So we have to take the positive one and you will obtain if you just do the calculations we will obtain X_e that is the equilibrium conversion is 0.963. So this is how we can solve using the stoichiometric table with a systematic approach. We can solve the different reactor problem very easily. Now in our next lecture we will start with the flow system. So thank you for hearing this lecture and we will continue our discussion in the next lecture.