Chemical Engineering Thermodynamics
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Lecture - 41
Chemical Reaction Equilibria

Hello and welcome back. We are talking about Chemical Reaction Equilibria in the previous two video lectures. We looked at what is known as the reaction coordinate, which will actually quantify all the mole fractions in a chemical reaction. And then we also looked at how we can calculate the equilibrium constant for a reaction. It turns out that the equilibrium constant is related to the Gibbs free energy change, in addition if we do not have the Gibbs free energy change for the reaction at the desired temperature, then we can use the heats of reaction data along with the specific heat capacities for each of the species to correct this equilibrium constant to the desired temperature.

What we will do today is work on a few problems on how to calculate this equilibrium constant, the numerical value for this equilibrium constant, and then apply the concept of equilibrium constant to calculate the mole fractions at equilibrium both for a gas phase reaction as well as for a liquid phase reaction.

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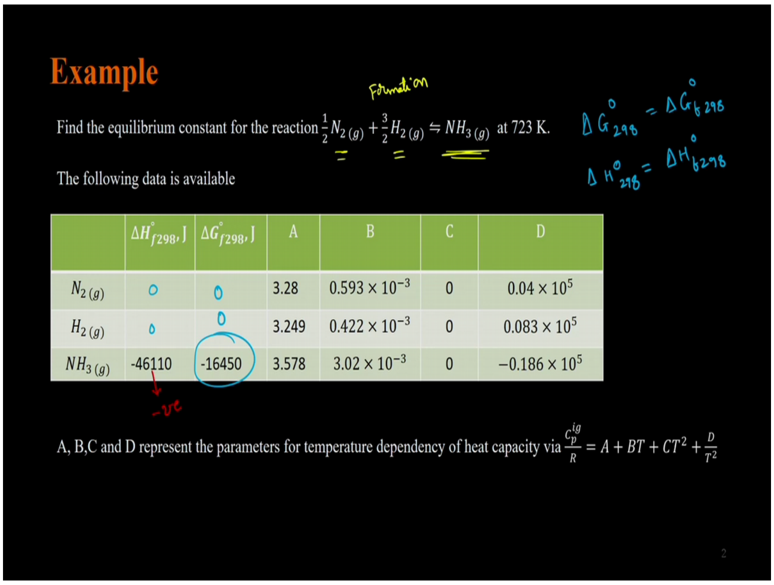

Example

Formation

Find the equilibrium constant for the reaction $\frac{1}{2}N_{2\,(g)} + \frac{3}{2}H_{2\,(g)} \leftrightharpoons NH_{3\,(g)}$ at 723 K.

$\Delta G^{o}_{298} = \Delta G^{o}_{f\,298}$

$\Delta H^{o}_{298} = \Delta H^{o}_{f\,298}$

The following data is available

	ΔH°_{f298}, J	ΔG°_{f298}, J	A	B	C	D
$N_{2\,(g)}$	0	0	3.28	0.593×10^{-3}	0	0.04×10^{5}
$H_{2\,(g)}$	0	0	3.249	0.422×10^{-3}	0	0.083×10^{5}
$NH_{3\,(g)}$	-46110	-16450	3.578	3.02×10^{-3}	0	-0.186×10^{5}

-ve

A, B,C and D represent the parameters for temperature dependency of heat capacity via $\frac{C_p^{ig}}{R} = A + BT + CT^2 + \frac{D}{T^2}$

So, let us get started then. The first problem for today is for synthesis of ammonia. This reaction is occurring at 723 Kelvin and we are interested in finding the equilibrium constant for this reaction at 723 Kelvin. We have some information given to us. First is the heats of formation data for ammonia, then the Gibbs free energy of formation, and also the specific heat capacities for each of the three species in the ideal gas state or rather the temperature dependency of the specific heat capacities for these three species of in the ideal gas state. So, we are going to use this data and calculate the equilibrium constant for the reaction.

Now, if you recall the equilibrium constant K is defined as the change in Gibbs free energy over rt or negative of that and then that would be ln K. But then since we require the equilibrium constant at 723 Kelvin, we need the Gibbs free energy change at seven twenty eight, the 723 Kelvin. Now, if we look at the data given to us, we were given the Gibbs free energy change not at 723 Kelvin, but rather at 298 Kelvin and also it is not a Gibbs free energy change, but only the Gibbs free energy of formation for ammonia.

Now, if you recall the way we have defined the formation reaction is it is the it is a reaction in which one mole of the desired species is formed from its constituent elements right. And in this case, in fact, the reaction we are looking at is the formation reaction for ammonia. We are making 1 mole of ammonia in this reaction all right, we are making 1 mole of ammonia in this reaction, and it is formed from its constituent elements, 2 moles of nitrogen or half a mole of nitrogen and 1.5 moles of hydrogen. So, in fact, this is the formation reaction for ammonia, and hence this number given to us negative 16450 is actually the Gibbs free energy for this reaction as well or Gibbs free energy change for this reaction as well.

Alternately if you think about it the Gibbs free energy for formation of the two species nitrogen and hydrogen is 0. And hence if you take the or if we calculate the Gibbs free energy of formation for this particular reaction, it is still going to be negative 16450 same thing for the enthalpy of formation. So, in that sense, these two numbers given here are not just heats of formation and Gibbs free energy of formation, they also turn out to be heat of the desired reaction and the Gibbs free energy change of the desired reaction for this particular scenario. Now, once we sorted that out let us see what else we need.

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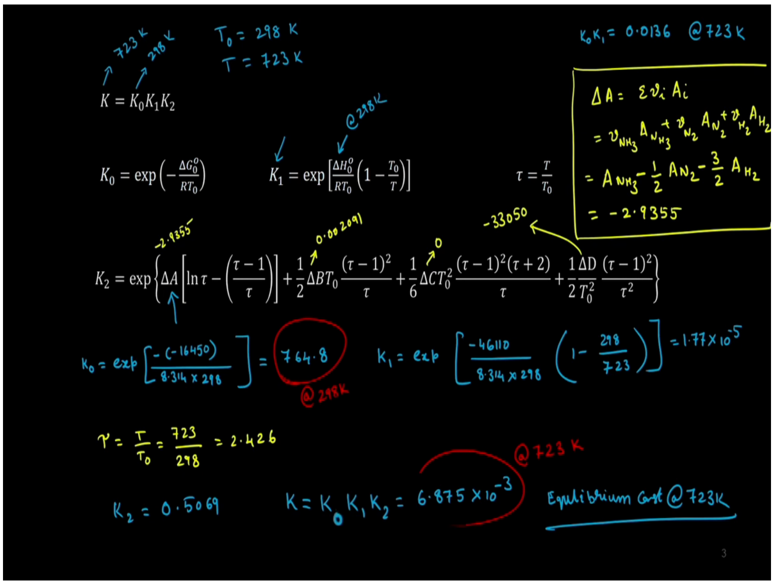

723 K 298 K

$T_0 = 298\ K$

$T = 723\ K$

$K = K_0 K_1 K_2$

$K_0 K_1 = 0.0136$ @723 K

$K_0 = \exp\left(-\frac{\Delta G_0^o}{RT_0}\right)$

@298K

$K_1 = \exp\left[\frac{\Delta H_0^o}{RT_0}\left(1 - \frac{T_0}{T}\right)\right]$

$\tau = \frac{T}{T_0}$

$\Delta A = \Sigma \vartheta_i A_i$

$= \vartheta_{NH_3} A_{NH_3} + \vartheta_{N_2} A_{N_2} + \vartheta_{H_2} A_{H_2}$

$= A_{NH_3} - \frac{1}{2} A_{N_2} - \frac{3}{2} A_{H_2}$

$= -2.9355$

-2.9355 0.002091 0 -33050

$$K_2 = \exp\left\{\Delta A\left[\ln\tau - \left(\frac{\tau - 1}{\tau}\right)\right] + \frac{1}{2}\Delta B T_0 \frac{(\tau - 1)^2}{\tau} + \frac{1}{6}\Delta C T_0^2 \frac{(\tau - 1)^2(\tau + 2)}{\tau} + \frac{1}{2}\frac{\Delta D}{T_0^2}\frac{(\tau - 1)^2}{\tau^2}\right\}$$

$K_0 = \exp\left[\frac{-(-16450)}{8.314 \times 298}\right] = 764.8$ @298K

$K_1 = \exp\left[\frac{-46110}{8.314 \times 298}\left(1 - \frac{298}{723}\right)\right] = 1.77 \times 10^{-5}$

$\tau = \frac{T}{T_0} = \frac{723}{298} = 2.426$

$K_2 = 0.5069$

$K = K_0 K_1 K_2 = 6.875 \times 10^{-3}$ @723 K

Equilibrium Cont @723K

So, we have the Gibbs free energy at 298 Kelvin, but what I need is the equilibrium constant at 723 Kelvin. In this scenario, this is at 298 Kelvin, so the temperature T naught we are looking at in all this equations is 298 Kelvin that is given to us. And if actual temperature of the reaction is 723 Kelvin, so we have to correct K from 298 to 723 Kelvin. The way we do that is using these two factors K 1 and K 2. K 1 turns out to be the correction factor is zooming that the enthalpy of the reaction is constant, this turns out to be the enthalpy at 298 Kelvin, and this is the value of course, at 298 Kelvin. And then the second correction is to correct for change in enthalpy itself with temperature. And the way we do it is using the specific heat capacities delta A, delta B, delta C and delta D right.

Now, so let us calculate each one of these terms. The first term K naught turns out to be exponential of negative delta G naught, which is negative of negative 16450 over r which is 8.314 times T naught which is 298. And if I calculate this number, it turns out to be 764.8, this is the value of K naught. This is the equilibrium constant if the reaction were to occur at 298 Kelvin. Top of this we correct it for K 1, the value would be exponential of delta H naught in this case delta of H naught is negative four 46110 over 8.314 times 298 that is T naught 1 minus 298 over 723. And if we simplify, this number turns out to be 1.77 into 10 power minus 5.

Now, if I just leave it at this and I calculate the product of the two terms K naught times K 1, then it would come out to be it would come out to be 0.0136, this is the value of K naught times K 1 at 723 Kelvin. But then this is assuming this will be the equilibrium constant, if we assume that this were delta H is constant with temperature which it is not we are given the specific heat capacity. So, what we do is employ another factor K 2 to correct for change in delta H with temperature. And the way we do that is using the expression given here.

And if you recall this delta A right, let me use another ink here delta A is sigma nu i A for i right. And what we are given is a specific heat capacities A, B, C or the terms for parameters for specific heat capacities A, B, C and D for each of the species. In that sense delta A is going to be nu for ammonia times A for ammonia plus nu for nitrogen times A for nitrogen plus nu for hydrogen times A for hydrogen.

And for ammonia nu is 1, it is a product. So, it is positive and it is one in this case. So, it will be A for ammonia. For nitrogen half a mole of nitrogen is reacting it is a reactant. So, it is negative and the stoichiometric coefficient is half negative half times A for nitrogen. And for hydrogen stoichiometric coefficient is negative 3 over 2 times A for hydrogen. And if I simplify all these numbers it turns out that the value what we get is the value of A. And in this case that number turns out to be two negative 2.9355.

And similarly I can calculate the other values this is negative 2.9355. I can calculate the value of B going by a similar logic, it would be 0.002091. In this case, C is 0 for all the species in any way. And finally, the value for D, we get going by similar logic is negative 33050 negative 33050. So, once I calculated delta A, delta B, delta C and delta D, I can calculate K 2 now right, K 2 is going to be all of these we also need to calculate tau right.

So, let us write tau down first. Let us write tau first. Tau is T over T naught. And in this case it is 723 over 298, and turns out to be 2.426. Once I have all of these numbers, I can go back and calculate K 2 plug in all the numbers and it turns out K 2, we get is going to be 0.5069. Once we have this K is going to be in this case this product turns out to be 6.875 times 10 to the power negative, negative 3. So, this is the equilibrium constant at 723 Kelvin.

Now, notice that delta H or notice that at 298 Kelvin, the equilibrium constant is 700 right, where was that yeah at 298 Kelvin the equilibrium constant is 764.8. But if I increase the temperature, the equilibrium constant has gone down and came to 6.875 10 to the power negative 3, it has gone down considerably almost an order of 6 orders of magnitude right, that is because the enthalpy of the reaction is negative. If the enthalpy of the reaction is negative, it means that the reaction is exothermic, heat would be liberated. And at higher temperatures the forward reaction is not favored because of the exothermicity, and hence the equilibrium constant, constant goes down.

Now, you can also obtain the same going through these calculations mathematically find K naught and then K 1. And then if you multiply the product of K naught and K 1, it would be lower than K naught itself or in that sense K naught K 1 is going to be less than 1, because delta H is negative, which means that the equilibrium in case of an exothermic reaction is going to shift towards the left. When we increase the temperature the equilibrium will shift towards the right in case of an endothermic reaction if I increase the temperature.

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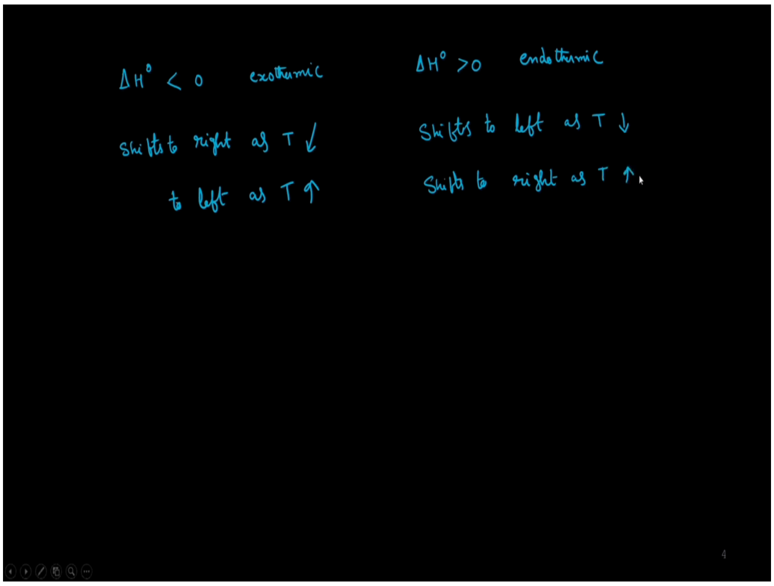

$\Delta H^{\circ} < 0$ exothermic

shifts to right as T ↓

to left as T ↑

$\Delta H^{\circ} > 0$ endothermic

Shifts to left as T ↓

Shifts to right as T ↑

So, what we said then is delta H naught less than 0 then it is an exothermic; and delta H naught greater than 0 then it is endothermic. The equilibrium shifts to right as temperature is decreased; it shifts to left as temperature is increased in case of an exothermic reaction. And in this case, the equilibrium shifts to left as temperature is increased is decreased; the equilibrium shifts to right as temperature is increased, this is the case for an endothermic reaction. And if you think about it this is what we call as Le

Chatelier's principle which we usually come across in physical chemistry this is where it comes from right.

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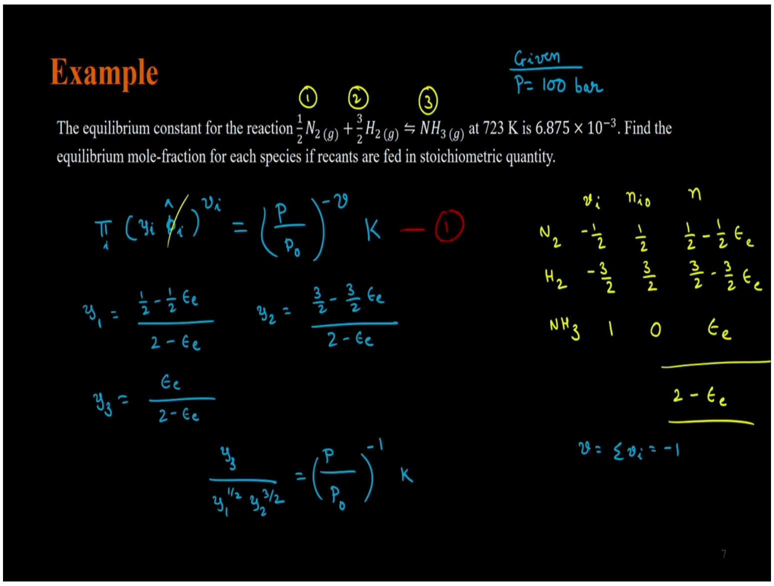

Example

Given

$P = 100$ bar

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The equilibrium constant for the reaction $\frac{1}{2}N_{2\,(g)} + \frac{3}{2}H_{2\,(g)} \leftrightharpoons NH_{3\,(g)}$ at 723 K is 6.875×10^{-3}. Find the equilibrium mole-fraction for each species if recants are fed in stoichiometric quantity.

$$\prod_i (y_i \cancel{\hat{\phi}_i})^{\nu_i} = \left(\frac{P}{P_0}\right)^{-\nu} K \quad - ①$$

	ν_i	n_{io}	n
N_2	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2} - \frac{1}{2}\epsilon_e$
H_2	$-\frac{3}{2}$	$\frac{3}{2}$	$\frac{3}{2} - \frac{3}{2}\epsilon_e$
NH_3	1	0	ϵ_e
			$2 - \epsilon_e$

$\nu = \sum \nu_i = -1$

$$y_1 = \frac{\frac{1}{2} - \frac{1}{2}\epsilon_e}{2 - \epsilon_e} \qquad y_2 = \frac{\frac{3}{2} - \frac{3}{2}\epsilon_e}{2 - \epsilon_e}$$

$$y_3 = \frac{\epsilon_e}{2 - \epsilon_e}$$

$$\frac{y_3}{y_1^{1/2}\, y_2^{3/2}} = \left(\frac{P}{P_0}\right)^{-1} K$$

So, let us move on to the second problem. In this case we have the same reaction. This time we are given the equilibrium constant at the desired temperature 723 Kelvin; if it is not given we know how to find it as in case of the earlier example. Once we know the equilibrium constant, the next thing we want to do is find the equilibrium mole fraction for each of the species right. And we are given the initial number of moles, we begin the reaction with and we want to find the equilibrium mole fraction or the mole fraction at equilibrium for each of the species.

Now, to solve this problem what we will do is we will use the given information. If you recall, what we said is that the product of the terms y i times phi i hat to the power nu i was P over P naught to the power negative nu times the equilibrium constant K. And for the special case of an ideal gas, we can neglect the fugacity coefficients as well. And once we do that what we get is simply the product of y i to the power nu i is P by P naught times negative nu multiplied with K or sorry P over P naught to the power negative nu multiplied with K.

Now, what we will do is, we will try to write the given information first. Let us write the three species here, ammonia, H 2, and NH 3. For each of these species nu i is negative half, negative 3 by 2 and 1. The initial number of moles is one-half for this, 3 by 2 for this and 0 for this right, that is how we are starting the reaction. And the final number of moles what we will do is we will write it in terms of the reaction coordinate. This would be half minus half times the reaction coordinate. This would be 3 by 2 minus 3 by 2 times the reaction coordinate, and this will be the reaction coordinate itself.

Now, at equilibrium, let us say that is when we say reaction coordinate, this is a reaction coordinate at equilibrium. Now, we will let us call it as epsilon e, it is not at any condition it is rather at the equilibrium conditions, so I am going to use the subscript e for this reaction coordinate. Now, at this react equilibrium condition if I add the total number of moles, it will be 2 minus this will be 2 times epsilon plus epsilon that would add up to 2 minus epsilon that is the total number of moles.

So, if I were to write the equilibrium mole fractions in terms of the reaction coordinate, then y let me label these species for sake of ease, I am going to call this as species 1, this as species 2, and ammonia as species 3. So, y 1 is going to be half minus half times epsilon at equilibrium by 2 minus epsilon; y 2 is going to be 3 by 2 minus 3 by 2 times epsilon over 2 minus epsilon; and y 2 is going to be y 2 is going to be epsilon over 2 minus epsilon right. Once we have these I can put these, I can rewrite the equation 1, this time in terms of the reaction coordinates rather than mole fractions.

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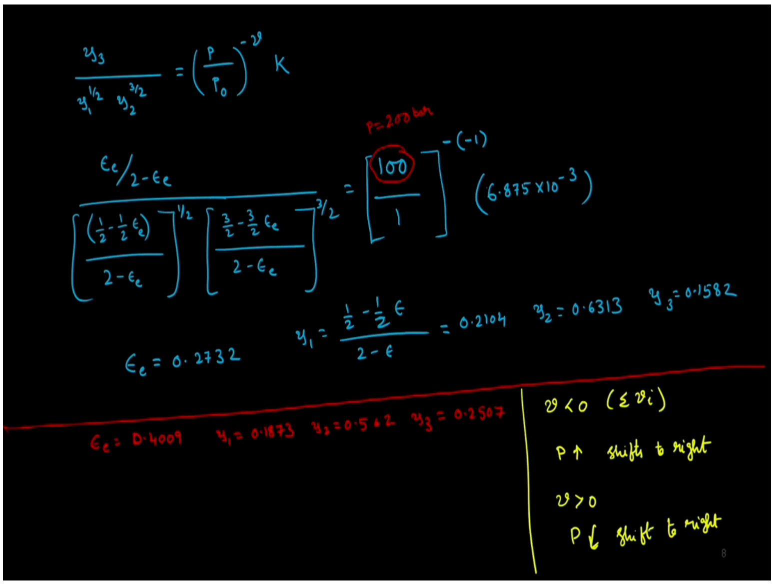

And when I do that what happens is. So, it reads y 2 by y 1 to the power half y 2 to the power to the power 3 over 2 is equal to p over p naught times negative nu times K that was the equation. I can rewrite all the y’s in terms of the equilibrium reaction coordinate that will become epsilon by 2 minus epsilon that is the y 3. Then y 1 is half minus half epsilon by 2 minus epsilon to the power half. And this will be 3 by 2 minus 3 by 2 times epsilon by 2 minus epsilon to the power 3 over 2. This will equal p which is 100. Well we are not given p for this particular problem. So, let us say we want to find the let us say the reaction is occurring at 100 bar, so let us pick a pressure for this reaction it should have been given.

So, let us say this is the given information along with everything else in the problem. So, the pressure for this particular reaction is 100 bar right in that case p over p naught is going to be 100 over p naught is the standard state pressure, and we said that for gases the standard state pressure is usually 1 bar that is what is chosen. And based on this standard state pressure, we obtained the Gibbs free energy of formation from which we obtained K data as in case of the previous problem. So, p naught is 1 bar in this case to the power negative, nu is negative 1, negative of negative nu. So, negative 1 is nu, negative nu is then negative of negative 1, which is going to be 1 times K. And, K in this case is given to us it is 6.875 into 10 power minus 3 times 6.875 into 10 power negative 3.

So, this is the equation we are looking at. I should have used a subscript e throughout for all the reaction coordinates. Now, if you look at this equation, everything in this equation is pretty much fixed except reaction coordinate. And once you solve this equation what we get is the equilibrium reaction coordinate. And it turns out at 100 bar, this value turns out to be 0.2732 all right. Once we have the equilibrium reaction coordinate, I can go back and calculate the mole fractions. In this scenario, the mole fraction y 1, if you recall we said is related to the reaction coordinate, we have this equation half minus half epsilon over 2 minus epsilon. And that value for 100 bar turns out to be 0.2104. Similarly, y 2 is going to be 0.6313, and y 3 is going to be 0.1582 all right.

Now, let us see what happens if I operate the reactor at a different pressure since we solve this particular problem for 100 bar. Let us quickly run through another calculation let us say the reactor instead of being operated at a 100 bar is operated at much higher pressure at 200 bar. If we do that, nothing changes until this point except in this particular equation instead of 100 bar for the pressure I need to replace it with 200 bar all right. And once I do that everything else stays the same that is the only place where pressure appears in this equation.

And now I need to solve a new equation for epsilon. If I solve this particular equation, it turns out that the epsilon equilibrium reaction coordinate I get in this particular scenario is going to be 0.4009 it goes up. And the values of y 1 is going to be slightly lower because epsilon has gone up; y 2 is also going to be a little lower 562; and y 3 because it is the product it will increase slightly to 0.2507. So, as you can see, once the pressure has increased, the equilibrium reaction coordinate has increased and the reaction has moved forward, and it has shifted to the right in this particular scenario.

Remember we discussed about Le Chatelier principle in case of temperature effect, in this case this is the effect of pressure on the reaction. This particular scenario as it turns out right, nu the overall stoichiometric number which is sigma nu i is less than 0 right. The total number of moles in the reaction go down as the reaction moves towards the right. And once that happens to increase the forward reaction or to shift the reaction towards right, we need to increase the pressure when nu is less than 0. Similarly, when nu is greater than 0, I need to decrease the pressure to shift the reaction to towards right.

And this is again is what we call as Le Chatelier principle, but this is where it comes from mathematically this is the effect of pressure on the reaction does the reaction shift forward or backward as I change the pressure that depends on the overall stoichiometric number nu whether it is negative or positive. In fact, if it is 0, then pressure will not have any effect on the equilibrium reaction coordinate. So, that completes this particular problem.

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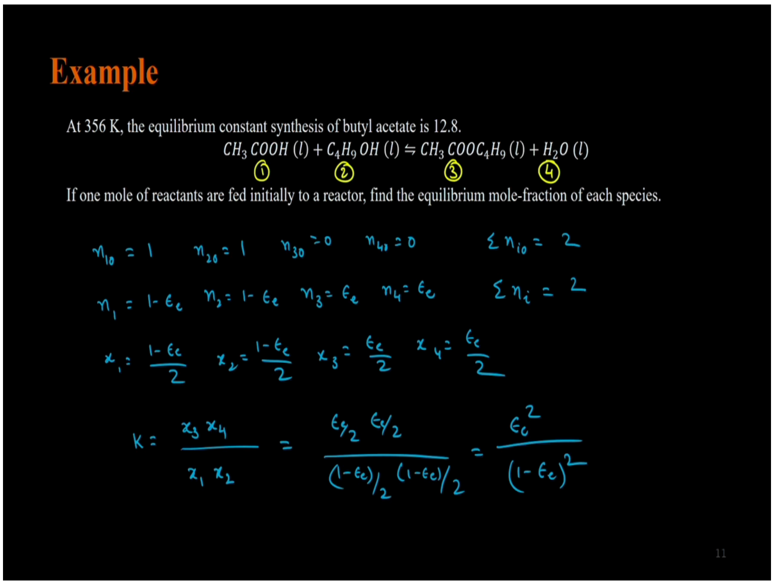

Example

At 356 K, the equilibrium constant synthesis of butyl acetate is 12.8.

$$\underset{①}{CH_3COOH\,(l)} + \underset{②}{C_4H_9OH\,(l)} \leftrightharpoons \underset{③}{CH_3COOC_4H_9\,(l)} + \underset{④}{H_2O\,(l)}$$

If one mole of reactants are fed initially to a reactor, find the equilibrium mole-fraction of each species.

$$n_{10} = 1 \quad n_{20} = 1 \quad n_{30} = 0 \quad n_{40} = 0 \qquad \Sigma n_{i0} = 2$$

$$n_1 = 1-\epsilon_e \quad n_2 = 1-\epsilon_e \quad n_3 = \epsilon_e \quad n_4 = \epsilon_e \qquad \Sigma n_i = 2$$

$$x_1 = \frac{1-\epsilon_e}{2} \quad x_2 = \frac{1-\epsilon_e}{2} \quad x_3 = \frac{\epsilon_e}{2} \quad x_4 = \frac{\epsilon_e}{2}$$

$$K = \frac{x_3 x_4}{x_1 x_2} = \frac{\epsilon_e/2\;\epsilon_e/2}{(1-\epsilon_e)/2\;(1-\epsilon_e)/2} = \frac{\epsilon_e^2}{(1-\epsilon_e)^2}$$

Let us see let us move onto one other problem ok. In this case, we have a liquid phase reaction. The reaction is for synthesis of butyl acetate from acetic acid and butanol we form butyl acetate and water. All of this is a liquid phase reaction occurring at 356 Kelvin and we are given the equilibrium constant for this particular reaction it is 12.8. Initially we feed 1 mole of each of the reactants to the reactor, what we want to find is the equilibrium mole fraction for each of the species. Again it is similar to the previous problem, but in this case instead of a gas phase reaction; this is a liquid phase reaction. Let us see how we can solve this particular problem.

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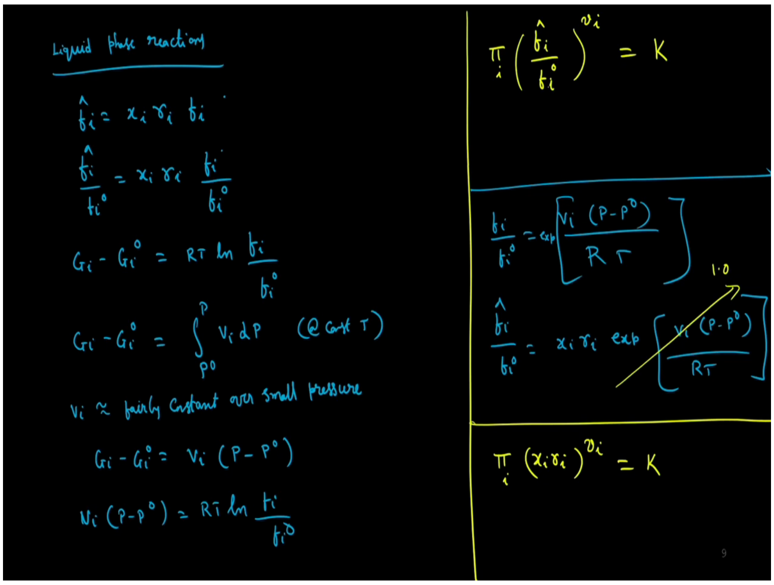

Liquid phase reaction

$$\hat{f}_i = x_i \gamma_i f_i$$

$$\frac{\hat{f}_i}{f_i^0} = x_i \gamma_i \frac{f_i}{f_i^0}$$

$$G_i - G_i^0 = RT \ln \frac{f_i}{f_i^0}$$

$$G_i - G_i^0 = \int_{P^0}^{P} V_i\,dP \quad (@\text{ const } T)$$

$V_i \approx$ fairly constant over small pressure

$$G_i - G_i^0 = V_i (P - P^0)$$

$$V_i (P - P^0) = RT \ln \frac{f_i}{f_i^0}$$

$$\prod_i \left(\frac{\hat{f}_i}{f_i^0}\right)^{\nu_i} = K$$

$$\frac{f_i}{f_i^0} = \exp\left[\frac{V_i (P - P^0)}{RT}\right]$$

$$\frac{\hat{f}_i}{f_i^0} = x_i \gamma_i \cancel{\exp\left[\frac{V_i (P - P^0)}{RT}\right]}^{\,1.0}$$

$$\prod_i (x_i \gamma_i)^{\nu_i} = K$$

Before we do that let us quickly talk a little bit about the liquid phase reactions. And the way we have done this for a gas phase reaction is starting from the equation that reads the product of the terms f i hat over f i naught raise to the power nu i equals K the equilibrium constant for the reaction. And then we manipulated f i hats and f i naughts to get things in terms of the mole fractions and hence the reaction coordinates. What we will do now is do a similar exercise. Let us first look at the ratio f i hat over f i naught. For a liquid phase mixture, f i hat or the fugacity of species i in the liquid is x i gamma i f i, where f i is the pure component fugacity.

So, this ratio then f i hat to f i naught is simply going to be x i gamma i f i over f i naught. So, using the activity coefficients, we have eliminated the need for fugacity of species in the mixture, now I have the ratio of the pure component fugacity at the condition of interest to the fuel component fugacity at the standard state. The way we will handle it is writing G i minus G i naught to be R T ln f i over f i naught right. And since G i minus G i naught is integral of p naught to p vi dp at constant temperature. Remember that G is vdp, so G i minus G i naught is that integral.

And if v i is fairly constant over small pressure changes, which might be true because this is a liquid mixture. So, we can neglect the change in the molar volume of the liquid mixture over small pressure changes. And if that happens V i can come out of the integral and G i minus G i naught is going to be V i p minus p naught. Now, I can take this put it back there, so that v i p minus p naught, then we will be RT ln f i by f i naught right.

So, allow me to use this space. What we will do then is write the ratio f i by f i naught as vi p minus p naught over RT in fact, exponential of this term this will be the ratio f i to f i naught from this particular expression. So, I will go back put it there what happens then is f i hat over f i naught is going to be x i gamma i exponential of v i p minus p naught over RT. Now, if you recall this is something similar something similar to the pointing correction factor. We talked about right.

This exponential term is similar to the pointing correction factor we talked about earlier in case fugacity of a pure liquid. For fairly small pressure changes again if p minus p and p naught are pretty close to one another, I can even neglect this term the pointing correction factors are going to be very small usually for conditions of interest, this term is going to be very close to 1, I can neglect that. And if that happens the ratio of f i hat to f i naught will be simply x i xi times gamma i. I can put this back in the equation above, and what happens then is pi or the product of the terms f i hat to f i naught will now be x i gamma i to the power nu i equals K.

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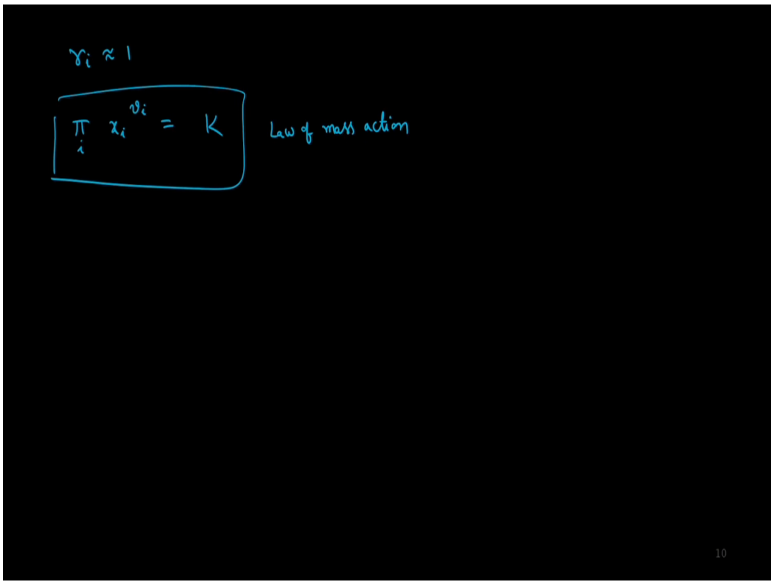

$\gamma_i \approx 1$

$$\boxed{\prod_i x_i^{\nu_i} = K}$$

Law of mass action

Now, for liquid mixtures which are ideal in nature, the activity coefficient also will be equal to 1, and that equation then reduces to the product of the terms x i to the power nu i will be simply equal to K right. And this is what we call as law of mass action in physical chemistry right. If it is not 1, then we also have to include the activity coefficient, and use the formulation here which reads the product of the terms x i gamma i to the power nu i will be equal to k. But if the liquid mixture is ideal, then I can simply use a law of mass action to handle the particular scenario.

Now, let us go back and look at a problem to apply this particular equation. We have a reaction which is used to synthesize butyl acetate, it is an esterification reaction, the reaction is between acetic acid and butanol to give butyl acetate and water. This is completely a liquid phase reaction occurring at 356 Kelvin, we are given the equilibrium constant K for the reaction is 12.8 at this temperature. Initially we are feeding 1 mole of each of the two reactants into the reactor, and we want to find the equilibrium mole fractions for each of the two species.

Let us see how we can solve this particular problem. Let us as we have done in the previous example, let us give some numbers for each of the species 1, 2, 3 and 4 right. The initial number of moles n 1 naught is 1; n 2 naught is 1; n 3 naught is 0; n 4 naught is also equal to 0. If the reaction proceeds, then the final number of moles is going to be 1 minus epsilon at equilibrium it will be epsilon e; this will be 1 minus epsilon e; this will be epsilon; this will also be epsilon.

Now, if I add this will be 2; and this will be 2, epsilons cancel, this will still be this will still be 2. The mole fractions y 1 is going to be 1 minus epsilon by 2; y 2 will also be 1 minus epsilon by 2; y 3 will be epsilon by 2; y 4 will also be equal to epsilon by 2 all right. And well I should have used the term x for mole fraction instead of y, because we are talking about a liquid phase reaction. So, let us call them as x 1, x 2, x 3 and x 4.

Now, for the liquid phase reaction, if I assume the solution to be ideal, then this is simply x 3, x 4, both 3 and 4 the products are new is of plus 1 and plus 1. The reactants of new is of negative 1, so they appear in the denominator it will be x 1 times x 1 times x 2. So, this will be epsilon over 2 epsilon over 2 or epsilon e rather over 2 1 minus epsilon e by 2 1 minus epsilon e by 2. So, this will be epsilon e square over 1 minus epsilon e square. This is the value for K right. We are already given the value of K.

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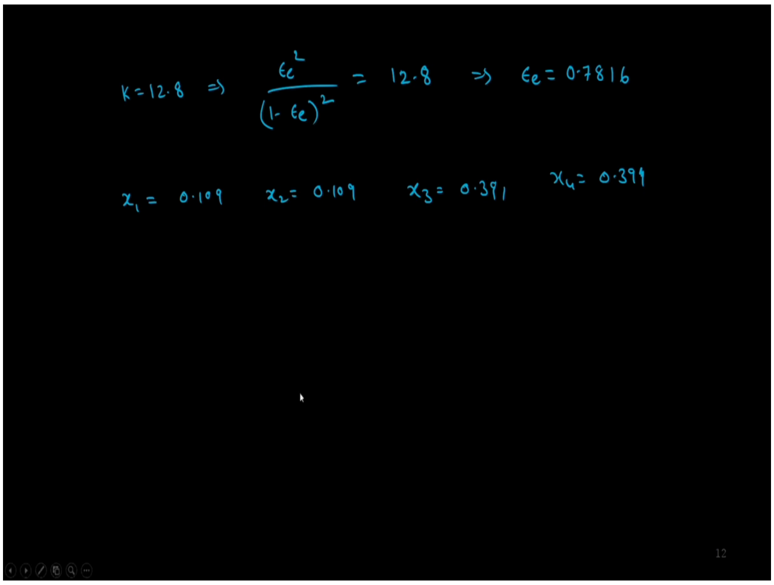

$$K = 12.8 \Rightarrow \frac{\epsilon_e^2}{(1-\epsilon_e)^2} = 12.8 \Rightarrow \epsilon_e = 0.7816$$

$x_1 = 0.109$ $x_2 = 0.109$ $x_3 = 0.391$ $x_4 = 0.399$

K is 12.8, so that implies at equilibrium epsilon e minus square by 1 minus epsilon e squared will be equal to 12.8. And if I solve this particular equation i get the reaction coordinate at equilibrium in this scenario it turns out to be 0.787816. Once I have the reaction coordinate finding the mole fractions is pretty straightforward in this scenario turns out that x 1 is 0.109, x 2 also is same 0.109; x 3 is 0.391 and so is x 4. So, what we have done in this particular problem is we have used the liquid phase reaction, we have used the, we have related the equilibrium constant in the liquid phase reaction to the equilibrium mole fractions.

Of course, assuming that the activity coefficient in the liquid mixture are 1, but it does not have to be if we know the activity coefficients, they can also be incorporated into these expressions and we can still solve the problem to obtain the conversion or the equilibrium reaction coordinate. And from that we can go back and calculate what each of the mole fractions at equilibrium are going to be. So, this is how we handle a liquid phase reaction. So, with that we conclude the video lecture today on chemical reaction equilibria that brings us to the end of this particular course on chemical engineering thermodynamics.