Material and Energy Balances
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Lecture - 62
Energy Balances on Reactive Processes - Part 5

Let us now continue with the second example problem.

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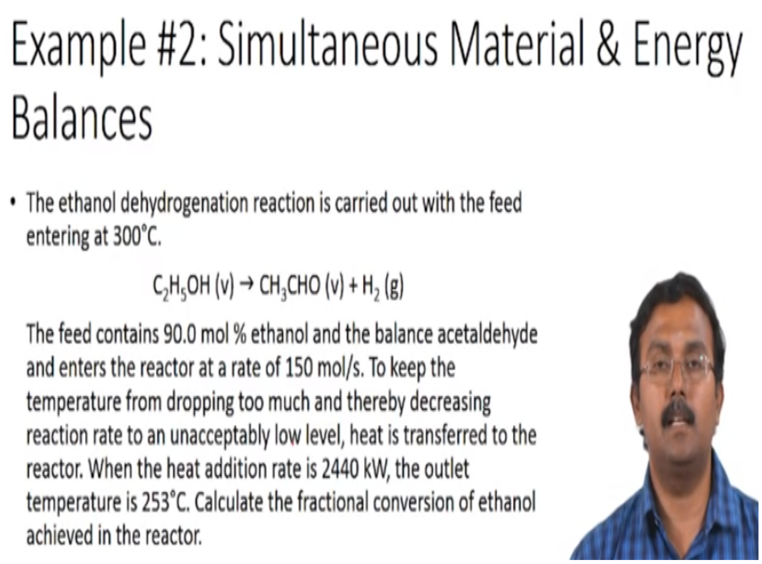

Here we will be performing material and energy balances simultaneously. As I had already said if you were to perform only material balances and use only equations from material balance you would end up with a degree of freedom which is greater than 0 which means you would not be able to solve the system. So however if you actually use the energy balance equation along with the material balance equations, you would be able to solve this problem.

Let us now look at the problem statement. The ethanol dehydrogenation reaction is carried out with the feed entering at 300 degree Celsius. Ethanol gives acetaldehyde and hydrogen. So the feed contains 90 mole percent ethanol and the balance is acetaldehyde and this enters the reactor at a rate of 150 mol/s. to keep the temperature from dropping too much and thereby decreasing the reaction rate to an unacceptably low level, heat is transferred to the reactor.

When the heat addition rate is 2440 kW, the outlet temperature is 253 degree Celsius. Calculate the fractional conversion of ethanol achieved in the reactor. So if you were to look at this problem and compare it with the previous problem which we solved, in the previous problem we were given the conversion. However, we were not given the exit temperature. Here we have actually been given the exit temperature but not the conversion.

We have been asked to calculate the conversion. So we can actually do this. We are trying to get this value. For this we will actually try to perform the energy balance and the material balance simultaneously. Unlike the previous problem where it was an adiabatic process, here heat is being transferred and the rate at which heat is transferred is also provided to you and this value can be used for the value of Q.

And you also have a mixture which is entering unlike the previous problem where you had only ethanol entering. So taking all these into account, let us now start solving the problem.

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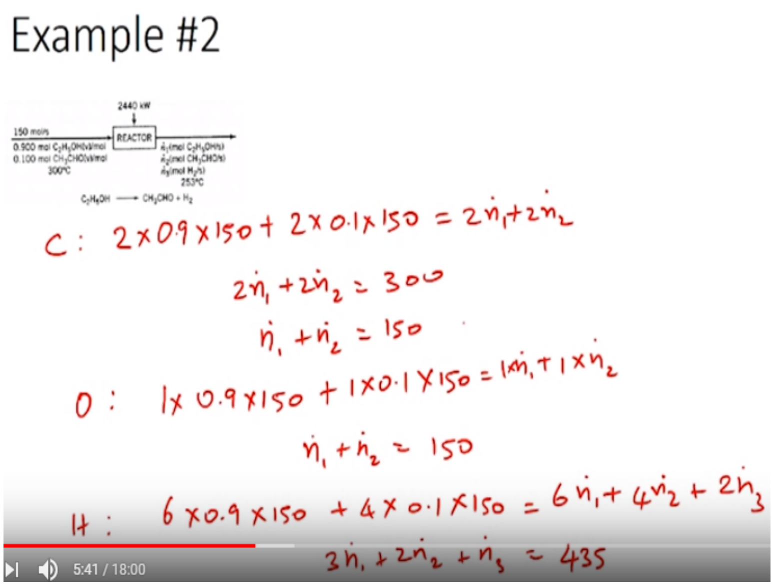

When we started the problem discussion said that here the degree of freedom would be greater than 0 if we did not have the energy balance equation. So to confirm that, let us now perform a degree of freedom analysis. So what are the variables which we have in this system? We have 3 unknowns. You have the molar flow rate of ethanol leaving the system, molar flow rate of acetaldehyde leaving the system and molar flow rate of hydrogen leaving the system.

We know how much of ethanol and acetaldehyde are entering. However, we do not know the composition of the exit stream at all. So we have 3 unknowns. So how many independent equations can we write? So if we were to write elemental balances, we would actually be able to write 3 equations, right? So we can write a carbon, hydrogen and oxygen balance. However, what you would see is oxygen and carbon balances are dependent on each other.

We can try writing the equations and see how that actually comes out. So the carbon balance for this system would be you have 2 atoms of carbon in every molecule of ethanol. So you would have 2 times 0.9 times 150 which is the number of moles of, number of atoms of carbon entering through ethanol plus two times 0.1 times 150 which is the number of atoms of carbon entering through acetaldehyde. So this would be the input term.

This would be equal to output. For an elemental balance as you know there is no generation or consumption terms and at steady state accumulation would also be equal to 0 so that is why we can directly write input equals output. So now let us see what the output equation would be. Output would be 2 n 1 dot + 2 n 2 dot. So this would mean that we are left with 2 n 1 dot + 2 n 2 dot = 300 right and the equation will simplify to n 1 dot + n 2 dot = 150.

So if you were to write an oxygen balance, then what would happen is, you would have 1 times 0.9 times 150 which is the number of atoms of oxygen entering along with in the form of ethanol. So 1 times 0.9 times 150 + 1 times 0.1 times 150 which is the atoms of oxygen entering in the form of acetaldehyde giving you an output stream which would be 1 times n 1 dot + 1 times n 2 dot. So the equation basically simplifies to again n 1 dot + n 2 dot = 150.

So you can write a hydrogen balance which would basically be 6 times 0.9 times 150 + 4 times 0.1 times 150 which = 6 times n 1 dot + 4 times n 2 dot + 2 times n 3 dot. So from this you can actually get an equation for the hydrogen balance which would simplify to 3 n 1 dot + 2 n 2 dot + n 3 dot = 435. So what you have is you have 3 elemental balance equations which you have written.

However, equations 1 and 2 are the same indicating that there are dependent equations and now you are stuck with 2 independent equations and 3 unknowns.

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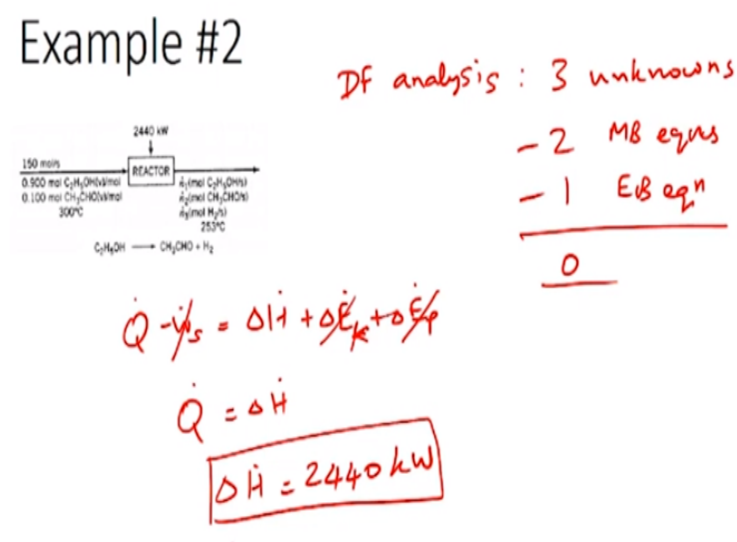

So if we were to perform the degree of freedom analysis, degree of freedom analysis would basically say that you have 3 unknowns and 2 material balance equations. So do you have anything else you can use? Yes, here you can use the energy balance. So we can actually get 1 energy balance equation and once we use that you actually have 3 equations and the degree of freedom now becomes 0. So with 0 degrees of freedom, we will be able to solve this system.

So for this we need to write the energy balance equation. So how do we go about preparing the energy balance equation? First thing is to identify what system it is. So this is an open system. You have material coming in and leaving. So you would start with the open system energy balance equation which is Q dot – W s dot = delta H dot + delta E k dot + delta E p dot. So here you do not have any moving parts. So shaft work will be 0.

You do not have any kinetic or potential energy changes. So the equation simplifies to Q dot = delta H dot and we will have to write this equation because once we prepare this equation you would actually have the molar flow rates of each of the components as part of the delta H dot and we will be able to solve for the values using the other 2 equations as well. So Q dot is already given to us as 2440. So we will use that value. So your delta H dot will simplify to 2440 kW.

So now we need to find out the equation which would represent delta H dot. So for that we would have to build the enthalpy table.

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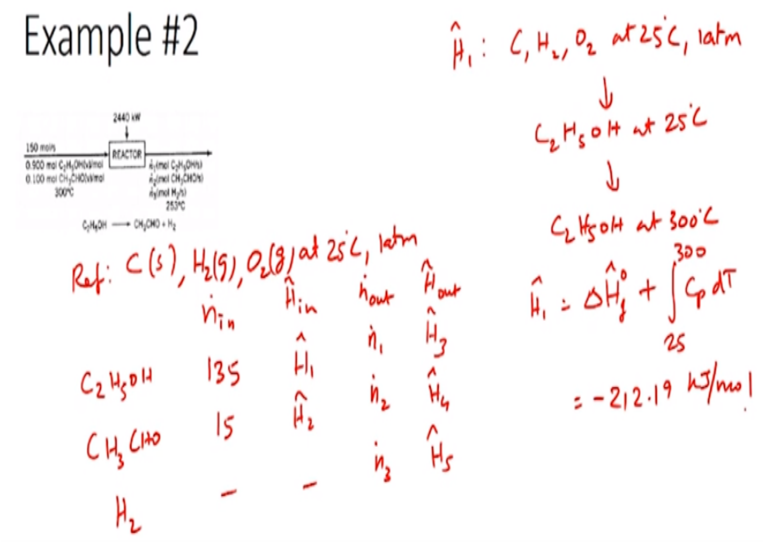

So let us identify the reference state which we would want to use. So here I have used the elements as the reference state so that I can use the heat of formation method. So going about that, what I would have is the reference states would be carbon solid, hydrogen gas and oxygen gas all at 25 degree Celsius and 1 atmosphere. So this would be my reference state. So now the substances which I have are C2H5OH, CH3CHO and hydrogen.

So I would have n dot H cap in, n out dot and H cap out. So what is the molar flow rate of ethanol in the system? So you have 150 mol/s of the mixture coming in. 0.9 of that is the mole fraction of ethanol in that mixture. So it will be 0.9 times 150 giving you 135. So the remaining is acetaldehyde. So 15 moles of acetaldehyde. There is no hydrogen entering.

So in the exit stream you have n 1 dot, n 2 dot and n 3 dot for each of the components which are leaving the system. We now need to identify the enthalpies for these components. So for ethanol you would have an enthalpy which needs to be calculated. We will call that H 1 cap and this would be H 2 cap. You do not have to worry about the enthalpy of hydrogen gas for the inlet stream. You would have H 3 cap, H 4 cap and H 5 cap, all needs to be identified.

So now let us see how we would go about calculating each of these enthalpies. So your H 1 cap is basically the process where carbon, hydrogen and oxygen in their native states at 25 degree Celsius and 1 atmosphere forms C2H5OH at 300 degree Celsius. So for this to take this into consideration, we have to look at two steps. The first would be the formation of ethanol and the second would be the heating of ethanol from 25 to 300 degree Celsius.

So you have this going to ethanol at 25 degree Celsius and then going to ethanol at 300 degree Celsius. So from here you can calculate H 1 cap, as the first step is the heat of formation. So the standard heat of formation for ethanol can be used for identifying the enthalpy of the first step plus integral C p of ethanol dT from 25 to 300 degree Celsius. So this would give you a value of -212.19 kJ/mol. So similarly we can calculate the values for H 2 cap, H 3 cap, H 4 cap and H 5 cap as well.

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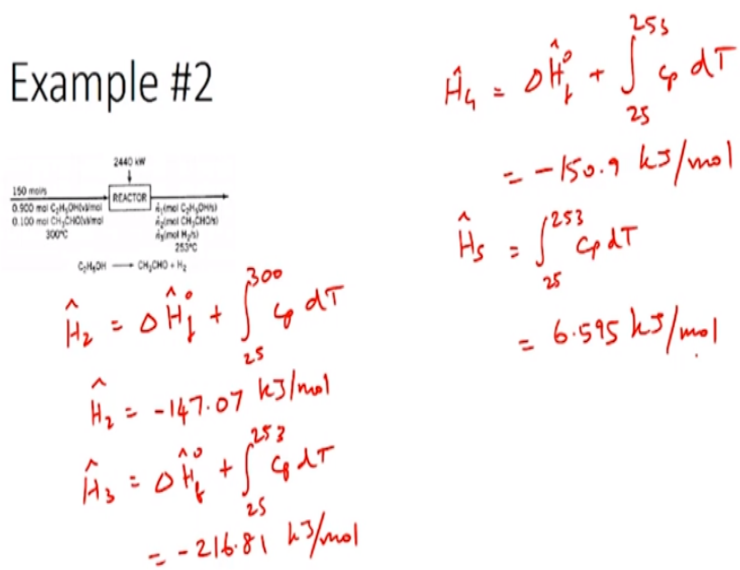

So let us go about doing each of them. So H 2 cap again is the process of formation of acetaldehyde from carbon, hydrogen and oxygen and then heating it from 25 degree Celsius to 300 degree Celsius. So you would have H 2 cap would be equal to the heat of formation of acetaldehyde, standard heat of formation of acetaldehyde plus integral 25 to 300 C p of acetaldehyde dT.

So using this equation and finding the values for heat of formation and the C p value for acetaldehyde vapor you would be able to substitute them and get the value of H 2 cap as -147.07. Now you have to again calculate H 3, H 4 and H 5 cap. So H 3 cap would again have 2 steps. First is the formation of ethanol from elements and the next is heating it from 25 degree Celsius 253 degree Celsius.

So you would have delta H f which is the standard heat of formation plus integral 25 to 253 C p of dT and this value can be calculated as -216.81 and all these are in terms of kJ/mol. So next thing is to calculate H 4 cap. So H 4 cap is again going to have heat of formation of acetaldehyde plus integral 25 to 253 C p of acetaldehyde dT. So this can be calculated as -150.9 kJ/mol. The last specific enthalpy that needs to be calculated is H 5 cap.

So this is for hydrogen. So here hydrogen is an element which means it would not have any heat of formation. So the only process you have is heating the hydrogen gas at 25 degree Celsius and 1 atmosphere which is the reference state to 253 degree Celsius which is the final condition. So you would have this as integral 25 to 253 C p of dT where C p is the C p of hydrogen gas. So you can calculate this as 6.595 kJ/mol.

So now we have all the values for H 1, H 2, H 3 and H 4 and H 5. So we can substitute this in the equation we had to get the third equation which is required for solving the material balances.

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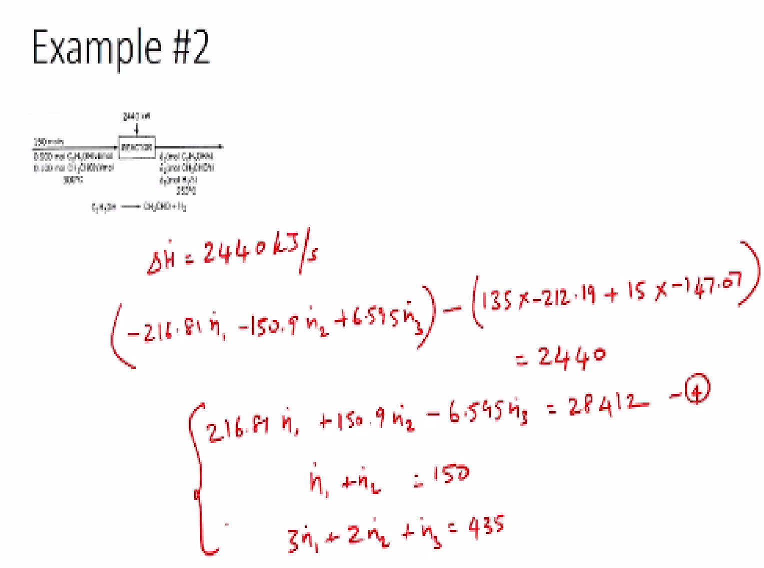

So now let us look at the equation. So we said that the equation simplifies to delta H dot = 2440 kJ/s. So if you were to plug the values for the enthalpies in the enthalpy table and calculate the change in enthalpy which is delta H dot. So this equation would become -216.81 n 1 dot – 150.9 n 2 dot + 6.595 n 3 dot. So this is the enthalpy of the outlet stream minus 135 times -212.19 + 15 times -147.07. This is the enthalpy of the inlet stream.

This would be equal to 2440 kJ/s. So you can simplify this equation and you would finally end up with the equation as 216.81 n 1 dot + 150.9 n 2 dot – 6.595 n 3 dot which would be = 28412. So this can be used as equation 4. So using equations 2, 3 and 4 we will be able to solve for n 1, n 2 and n 3. So the other equations we had were n 1 + n 2 = 150 and 3n 1 dot + 2n 2 dot + n 3 dot = 435.

So using these 3 equations and solving them simultaneously we can get the values for n 1, n 2 and n 3. Once we know these values, we can calculate the conversion of ethanol.

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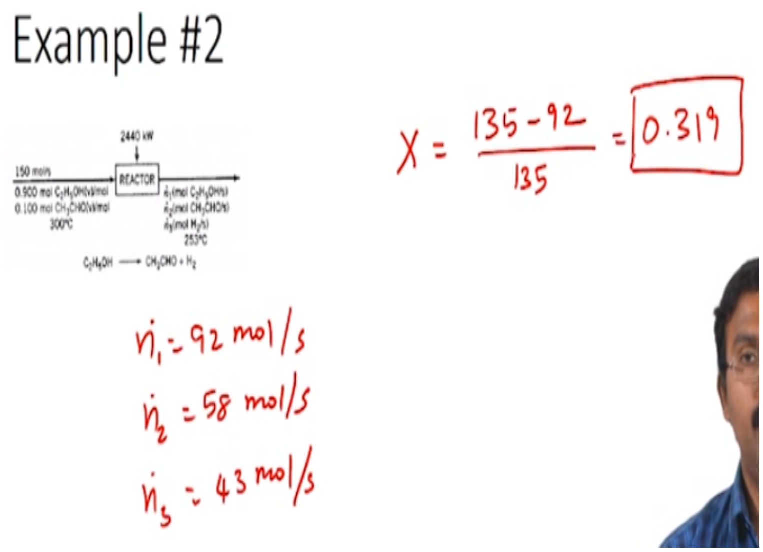

Solving these equations simultaneously, we would get n 1 dot = 92 mol/s; n 2 dot = 58 mol/s and n 3 dot = 43 mol/s. So we need to calculate the conversion of ethanol. So conversion is defined as amount consumed divided by amount fed. So if you want it to be in terms of percentage, we will multiply it with 100. So here it would be conversion x would be = 135 – 92 which is the consumption of ethanol. Input is 135, 92 is the output.

So you have the difference between them as the consumption and you have this divided by the feed which is 135 and you would get a conversion of 0.319 and this would be the conversion. So fractional conversion for ethanol is 0.319. So with this we have been able to perform a material balance calculation using the energy balance equation as one of the independent equations while we perform the calculations.

So this is a simultaneous material balance and energy balance calculation that has been performed together so that we can get the parameters we are looking for.