Material and Energy Balance Computations
Prof. ARNAB ATTA
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur

Lecture –24
Reactive Process Balance (Contd.,)

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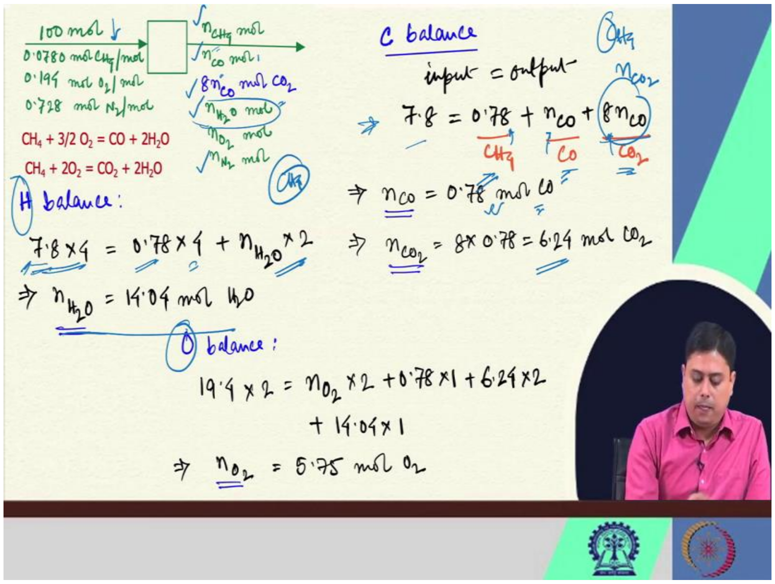

100 mol

0.0780 mol CH_4/mol

0.194 mol O_2/mol

0.728 mol N_2/mol

n_{CH_4} mol

n_{CO} mol

$8n_{CO}$ mol CO_2

n_{H_2O} mol

n_{O_2} mol

n_{N_2} mol

$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

H balance:

$7.8 \times 4 = 0.78 \times 4 + n_{H_2O} \times 2$

$\Rightarrow n_{H_2O} = 14.04$ mol H_2O

C balance

input = output

$\Rightarrow 7.8 = \underbrace{0.78}_{CH_4} + \underbrace{n_{CO}}_{CO} + \underbrace{8n_{CO}}_{CO_2}$

$\Rightarrow n_{CO} = 0.78$ mol CO

$\Rightarrow n_{CO_2} = 8 \times 0.78 = 6.24$ mol CO_2

O balance:

$19.4 \times 2 = n_{O_2} \times 2 + 0.78 \times 1 + 6.24 \times 2 + 14.04 \times 1$

$\Rightarrow n_{O_2} = 5.75$ mol O_2

Hello everyone, welcome back once again in the NPTEL online certification course on Material and Energy Balance Computations. We were learning the reactive process balances. Now in the last class we started a problem that had a flow sheet like this that we had 2 multiple reactions in which the methane had an incomplete combustion and was producing carbon monoxide, carbon dioxide and water at the output.

In the output we had a known molar ratio of carbon monoxide and carbon dioxide we also knew the percentage conversion of methane. We applied degree of freedom analysis using all the 3 methods that we have learnt that is the molecular species balance, atomic species balance and extent of reaction and using molecular species balance we solved this problem. We have seen the application of molecular species balance for this problem and now we apply atomic species balance to solve this problem.

So, now in atomic species balance if you remember while doing the degree of freedom analysis we realized that in this case we have 3 atomic species independent as atomic species on which we can apply the balance. Now here we apply the balance on the atomic carbon atomic hydrogen and atomic oxygen. You must not confuse this with the oxygen balance because if we see the oxygen balance we have molecular species oxygen, oxygen as molecular species that we must not forget.

So, we have to be very specific in the terminology that is the atomic oxygen balance atomic hydrogen balance and atomic carbon balance. So, to start with we can do it for carbon balance. Now this reason behind the choice of carbon you can look at the problems or the flow sheet here and you can identify that the carbon is there in one input species the molecular species that is methane. In the output we had 3 molecular species where the carbon is appearing.

Similarly if you look at oxygen, oxygen here is appearing in at molecular species oxygen molecular oxygen we have carbon monoxide, we have carbon dioxide water as well as the molecular species oxygen. So, which means the number of appearance in the right and the left hand term are higher than the carbons because eventually we have to write input = output. So, although the input has one term on the right hand side and the output terms you have multiple appearance of oxygen atomic oxygen.

In case of hydrogen we see it also appears on the left hand side that is the input one time on the right hand side we have one that is in methane in water that is 2 times. So, we can either start with the carbon or hydrogen balance. Now here I have shown as the carbon balance which is the input = output. Now although here carbon is appearing 3 times do not forget that we have already calculated the methane, number of methane moles from the molecular species balance.

From molecular species balance we have calculated the number of nitrogen and from the percentage methane conversion we have already calculated the value of nCH_4. So, which means even for carbon we have only 2 unknowns on the right hand side and these 2 unknowns are further related by their molar ratio. So this is why the logical choice of sequence of solving this problem or to apply the balance is carbon at first.

So, here we have input = 7.8 moles because it is 7.8% of methane in the feed and one mole of methane contains one mole of atomic carbon. So, we have 7.8 moles of input that is we have the amount of mole that methane that goes out and there also we have each mole of CH_4 contains one mole of atomic carbon. So, which is the same that is 0.78 that we calculated in the last class that we have shown it.

From CO we can see that one mole of CO again contains one mole of atomic carbon and so as the carbon dioxide. Now these are the moles at the output. So, we have nCO + 8 × nCO because this is the nCO_2. So, these are the sources that are written here the source of atomic carbon in the output 0.78 comes from methane nCO comes from the carbon monoxide, 8 × nCO comes from the carbon dioxide.

So, now if we write the numeric and solve it we can easily find out what is the value of nCO because here in this equation we have only one unknown. So, we can quickly find out that the number of moles of carbon monoxide is 0.78 mole of carbon monoxide which is same that we calculated in the molecular species balance. So, as the carbon dioxide it is the 8 times of that mole. So, we have applied carbon balance the next is the hydrogen balance.

So, in hydrogen balance similar to this concept that is here in atomic species we need not consider about whether it is consumed whether it is generated it is simple input = output. The hydrogen input is happening through methane where we know the amount of methane and one mole of methane contains 4 mole of atomic hydrogen. So, this is multiplied by 4 this is the amount of methane.

The moles of methane in the outlet × 4 because as the reason I said it is CH_4 and the water one mole of water contains 2 moles of atomic hydrogen in the output we have nH_2 unknown quantity. So, multiplied by 2 we will have the amount of hydrogen atomic hydrogen that leaves the reactor. So, which means we have nH_2O = 14.04 mole which is again identical to our previous solution.

So, we knew nCH_4, nN_2 we calculated nCO, nCO_2, nH_2O the remaining part is nO_2 for that we apply the oxygen balance atomic oxygen balance and that is why it is written as simple O it is simple H by the same logic of input = output, input is happening through the atom molecular species of oxygen or oxygen at the molecular species and one mole of oxygen molecule contains 2 moles of atomic oxygen.

So, it is the amount here is 0.194 × 100 is the amount of molecular oxygen that goes into the system that × 2 is the amount of atomic oxygen goes into the system in the output we have the amount of oxygen that leaves the system multiplied by 2 this is the amount of atomic oxygen that goes in terms of nO_2 × the amount that we have here is for nCO that is with carbon monoxide one mole of carbon monoxide contains one mole of atomic oxygen.

So, that amount multiplied by one, one mole of CO_2 contains 2 moles of atomic oxygen. So, the amount of CO_2 × 2 this is the amount of atomic oxygen leaving the system as CO_2 + the amount that we have with water. So, oxygen is leaving in terms of molecular oxygen, carbon monoxide, carbon dioxide and this is water we know the amount of water leaving the system and one mole of water contains one mole of atomic oxygen.

So, here everything is known except nO_2, which we calculate as 5.75 mole of oxygen. So, which means like the previous solution by molecular species balance here we have all the moles the number of moles are known to us which are the identical values as of the molecular species balance. So, similarly once we have calculated the number of moles for all the species we calculate n_{total} for all the n_i the summation of n_i and then individual species divided by n_t is × 100 is our molar percentage for the molar composition of the outlet stream.

So, which means we have now seen the reactive process balance where multiple reactions are involved using atomic species balance and we can now clearly distinguish that how easy it is than the previous approach of molecular species balance.

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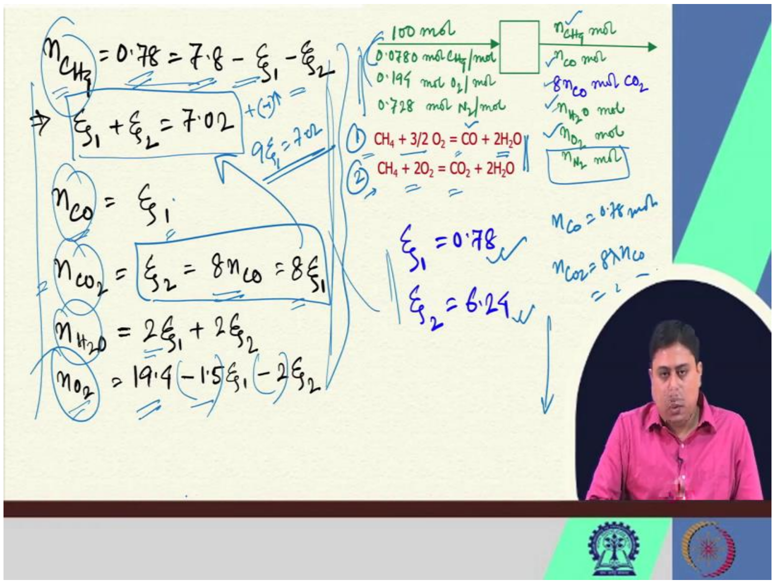

$n_{CH_4} = 0.78 = 7.8 - \xi_1 - \xi_2$

$\Rightarrow \boxed{\xi_1 + \xi_2 = 7.02}$

$+(-1)$

$9\xi_1 = 7.02$

$n_{CO} = \xi_1$

$n_{CO_2} = \boxed{\xi_2 = 8n_{CO} = 8\xi_1}$

$n_{H_2O} = 2\xi_1 + 2\xi_2$

$n_{O_2} = 19.4 - 1.5\xi_1 - 2\xi_2$

100 mol

0.0780 mol CH_4/mol

0.194 mol O_2/mol

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n_{CH_4} mol

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$8n_{CO}$ mol CO_2

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① $CH_4 + 3/2\ O_2 = CO + 2H_2O$

② $CH_4 + 2O_2 = CO_2 + 2H_2O$

$\xi_1 = 0.78$

$\xi_2 = 6.24$

$n_{CO} = 0.78$ mol

$n_{CO_2} = 8 \times n_{CO}$

Coming to the extents of reaction the same problem we can write the extent of reaction expressions for the 5 species that we have the 5 species are methane, carbon monoxide, carbon dioxide, water, oxygen the nitrogen is the non-reactive species for which we have separately encountered – 1 value because it is a independent non-reactive species in the system. So, here are the 5 expressions based on our understanding by designating this as the first reaction and this as the second reaction.

So, for the first reaction ξ_1 is the extent of reaction now we can see that the moles of methane going out of the system is 0.78 that we have calculated already based on the percentage conversion of methane that equal to the input amount of it which is 100 × 0.078 + the stoichiometric coefficient of – 1 because it is a reactant in the first reaction × the extent of reaction.

So, that is why it is $-\xi_1$ and for the same reason it is $-\xi_2$ for the second reaction. So, which means $\xi_1 + \xi_2$ = this value 7.02 is the first equation that we get. When we apply it for carbon monoxide it is generating only in the first reaction the feed does not contain any carbon monoxide. So, it is only ξ_1 because it has a stoichiometric coefficient of one and it is a product. So, it is positive one. So, nCO is ξ_1.

Similarly for carbon monoxide it is ξ_2 now nCO and nCO_2 we have a relation of 8 × nCO that means ξ_1 and ξ_2 are related by this relation. We apply it for water, water is the product in both the reactions without any input in the system. So, which means we have it is the $2 \times \xi_1$ because it has a stoichiometric coefficient of 2 in both the equations and those are the products so, + 2 + 2 in both the cases.

And for oxygen it is a reactant for both the reactions with an input amount of 19.4 – 3 / 2 in the first reaction this is the stoichiometric coefficient and – 2 for the second reaction that comes from the stoichiometry of the reaction. So, which means we have these relations and easily we can now find out what is the value of ξ_1 and ξ_2 because we have a relation ξ_1 and ξ_2 it is 8 times of that we replace it here.

So, it becomes $9 \times \xi_1 = 7.02$ which means ξ_1 and ξ_2 are known to us. Once it is known, we go back to these expressions to find out the value of each and every parameter which means nCO is 0.78 mole nCO_2 is 8 × of nCO. Similarly we calculate and we get the exact same value that we got in the last 2 methods that is the atomic species balance and molecular species balance.

So, this means that for a particular problem we have applied all the 3 methods and we have seen that it is apparent the molecular species balance is bit complexer than the other 2 methods, atomic species balance is the straightforward way and it appears to be a simple one than the other 2. So, I hope with this understanding you can apply this knowledge to solve any reactive system.

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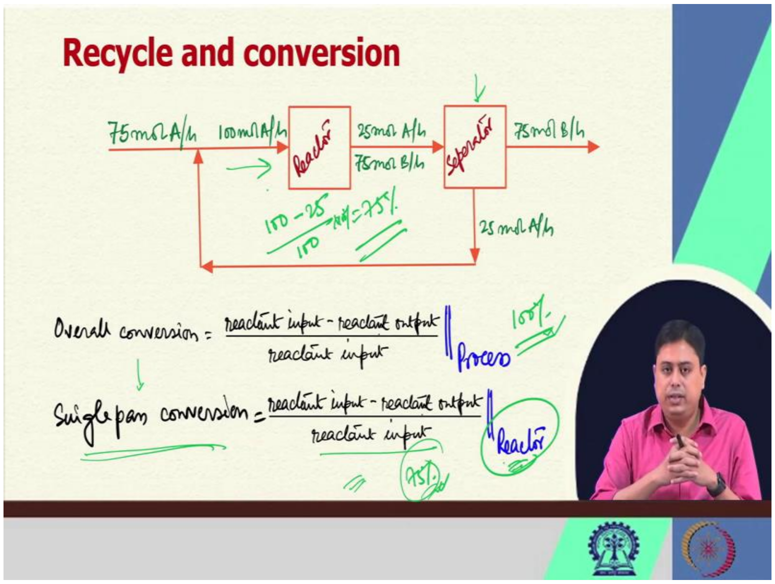

Recycle and conversion

$$\text{Overall conversion} = \frac{\text{reactant input} - \text{reactant output}}{\text{reactant input}} \quad \| \text{ Process} \quad 100\%$$

$$\text{Single pass conversion} = \frac{\text{reactant input} - \text{reactant output}}{\text{reactant input}} \quad \| \text{ Reactor} \quad 75\%$$

Now, although this example that we have seen is a single unit system. Now we have solved the non-reactive system for multiple units. The similar scenario would appear for the reactive system as well where we will have recycle or bypass. The approach will be exactly similar to that of the non-reactive species, that means when there is a recycle stream we have to consider the recycle part as a subsystem or a unit if it is an overall process.

This should be a mixing point when the fresh feed and the recycle stream mixes. So, we will have several sub section or sub units of a unit or the complete process or you can consider those as units of an overall process and we apply the similar way that we did for the multiple system in non-reactive case that first for each and every unit of a multiple unit process, We do the degree of freedom analysis we realize that which unit we have to take first to start solving the problem and subsequently we go to the other units.

Now in this case this is this example is shown for the recycle. Now since here the reactions are involved we will have the term called the conversion and there can be 2 different terms one is the overall conversion the other one is the single pass reactor conversion. Now here if you notice in this flow diagram what we have that a fresh feed of 75 moles of A per hour is coming into the system it goes to the reactor certain more amount of product that is B is formed.

It is separated in a separator the reactant is separated from the product and is recycled and mixed with the fresh feed. So, again the mixture of the fresh feed and the recycle stream is 100 mole per hour and the product leaves the system as 75 mole of B per hour. So, that means here we are considering the simple system. So, here the recycle stream is there as I just mentioned for the recycle stream you need to consider the mixing point for the bypass stream.

You have to consider a fractionating point and you have to apply the degree of freedom analysis for each and every subsystem. Now here if you look at the overall system that is this overall process we see A goes into the system the reactant goes into the system and only product B that is coming out although in the reactor subsystem all A is not converted the amount of A has been converted here is 75 mole of A the 25 mole is leaving the reactor.

And that is where two definition of conversion comes into play one is the overall conversion, overall conversion with respect to the process for the overall process that means the reactant input – reactant output divided by the reactant input. This is the overall conversion that means the conversion of reactant in the process the overall process with respect to process or specifically you can write the reactant input to the process – reactant output from the process divided by the reactant fed to the process.

This ratio is the overall conversion of the reactant which is in this case is 100%, the reactant input we have 75 because this is the system boundary for the overall process reactant output is 0 divided by 75. So, the overall conversion in this process is 100%. However the single pass reactor conversions that we call the single pass conversion and that happens with respect to the reactor. In that case the definition is reactant input to the reactor – reactant output from the reactor divided by the reactant input to the reactor.

Which is in this case we have 100 – 25 divided by 100, which is 75 × 100% it is 75 percent. So, the overall conversion of reactant A is 100% for the system. But the single pass conversion of reactant A is 75%. So, which means if you think it in this way that the overall conversion is improved because you have a separator which separates the unreacted component or unreacted reactant completely and recycled back to mix with the fresh feed that is how you achieve 100% reactant conversion for the overall process.

But at the reactor level you will always have a lesser amount of conversion than the overall conversion. This number would always be lesser than the overall conversion for any system. Now the point is you can operate the reactor with a low efficiency that means at a lower conversion rate and then you can place a separator high efficiency separator to separate the unreacted reactant which may be precious and recycle back to the reactor.

By this way you can improve the overall efficiency and also you can increase the high throughput to the reactor that means the high flow rate to the reactor the reactor can process a higher amount with a lower conversion rate but for a higher conversion the reactor may have to be operated at a lower flow rate. So, depending on your need and the final economic analysis that whether the placement of separator is economical than the high throughput of the reactor or say the low throughput of the reactor this comparative analysis will tell us that which one is beneficial whether we have to place a high efficiency reactor or we have to focus more on the high efficiency separator.

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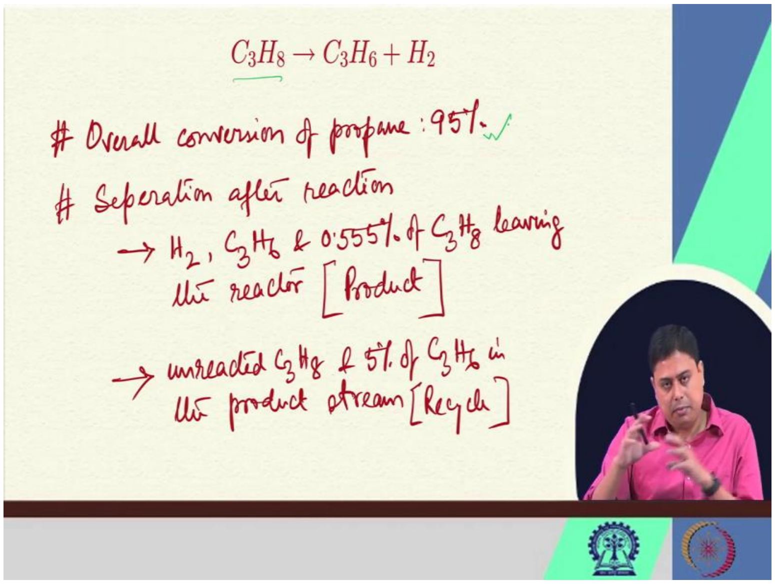

$$\underline{C_3H_8} \rightarrow C_3H_6 + H_2$$

\# Overall conversion of propane : 95% ✓

\# Seperation after reaction

→ H_2, C_3H_6 & 0.555% of C_3H_8 leaving the reactor [Product]

→ unreacted C_3H_8 & 5% of C_3H_6 in the product stream [Recycle]

So, the point is with this understanding we will solve a problem in the next class and the statement is something like this that we have propane the dehydrogenation of propane going to propylene and hydrogen. We know the overall conversion of propane this information is known to us and after the conversion is happening we are placing that in a separator the complete product stream that the stream that comes out from the reactor.

This is then separated in 2 streams one is the product stream the other one is the recycle stream the composition of the product stream is known and the recycle stream certain portion of its is known or basically the known thing is that the components are known that what is in the product stream and what are the components in the recycle stream we have to find out all the unknown variables in the system.

And specifically say the recycle ratio and the single pass conversion these 2 things. So, we will take up this problem in the next class and we will see how it is solved and the understanding of single and the overall conversion whether it is clear to us or not. With this I stop here and will see you in the next class, thank you for your attention.