Material and Energy Balance Computations
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Lecture –25
Reactive Process Balance (Contd.,)

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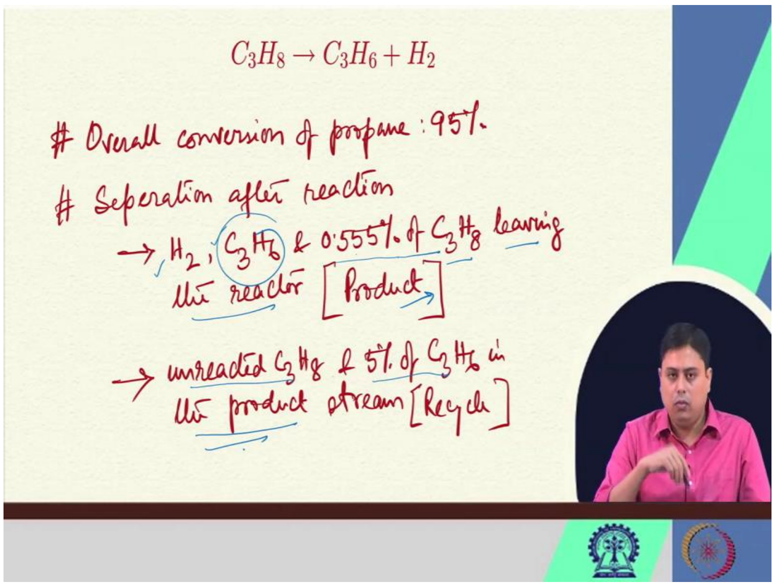

Hello everyone, welcome back once again in NPTEL online certification course on Material and Energy Balance Computations, we were in reactive process balance and in the last class I showed you this problem statement which we will solve today. So, the problem statement let me repeat it once again is that the dehydrogenation of propane to propylene. Now here it is happening in a reactor the overall conversion of propane is known to us which is 95%.

Once it leaves the reactor, the stream that leaving the reactor is separated and this after separation we have 2 streams one is the product stream that is taken out of the system the other one is recycled and mixed with the fresh feed, the product stream contains hydrogen, propylene and information given is that 0.555% of propane leaving the reactor. So, the amount of propane that is leaving the reactor of which 0.555% is going as the product or with the product stream.

The recycle stream is the unreacted reactant which is propane and 5% of propylene in the product stream that means whatever the amount is here its 5% is there in the recycle stream. So, these 2 are the information we can think of these are the additional information that are given here now these are important to identify because with the help of this information we can do the degree of freedom analysis.

Now as I mentioned that for multiple reactions and we have seen in general atomic species balance is a simple and straightforward approach. So, we will go with that.

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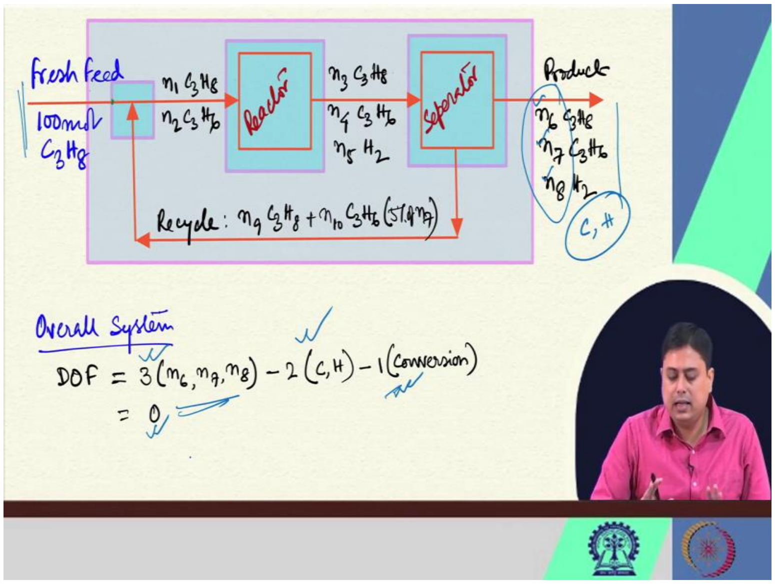

Now for this at first we have to draw the flowchart we have to label it, we have to identify the number of unknowns. Now from the previous example that we have seen where we applied 3 methods molecular species balance, atomic species balance and extent of reaction to a single unit reactive process. This you can think of an example in multiple unit reactive process where we are applying atomic species balance and here only one reaction is happening.

So, here we have fresh feed and our basis of calculation is 100 mole of C_3H_8 which is propane it is going into the reactor the reactor output is going into a separator. The separator separates its n_2 streams one is product stream the other one is the recycle stream. The recycle stream is mixed with the fresh feed and goes into the reactor. So, here the unknown components are identified everything here in one mole n_2 mole and for the sake of cleanliness here the moles are not written but you must follow that you have to write any number with its unit.

For the clarity it is just written as n_1, n_2, n_3, n_4, n_5 like this it should have been n_1 mole of C_3H_8 n_2 moles of C_3H_6. So, coming to this solution first of all we now understand that we have fresh feed with this we have recycled stream is mixed and this junction or the mixing point is highlighted. So, the highlighted boxes you can see there are 4 highlighted boxes one is the overall system the other 3 are the sub units.

One is the mixing point, one is the reactor and one is the separator just like we did for the non-reactive multiple unit processes. Here we know the product stream it is mentioned and those are the unknowns that we have that we have n_6, n_7, n_8 the sequence is has started from left to right. So, that that is why it is n_1, n_2, n_3, n_4, n_5, n_6, n_7, n_8, n_9 and n_{10} all are mole.

Now these numbers these nomenclatures can vary individual to individuals. So, here we have a C_3H_8 propane, propylene and hydrogen that is mentioned in the problem statement the recycle stream is having unreacted propane and certain percentage of propylene and the relation is given because if it is n_7, 5% of n_7 is there which means n_{10} is basically 0.5 of n_7 this relation is known to us and so, as the relation between n_6 and n_3.

Because it is mentioned in the problem statement that 0.555% of propane leaving the reactor that is there in the product stream. So the product stream leaving the reactor is this one in which we have n_3 amount of C_3H_8 and in the product stream we have n_6. So, which means we know a relation between n_3 and n_6. So, it is better to write here that we have a relation known with the n_3. So, now if we do the degree of freedom analysis by atomic species balance for the overall system this is what we did for the multiple units in non-reactive process.

So, for the overall system we identify that the unknowns are basically n_6, n_7, n_8 these are the product and this is known because we have assumed the basis of calculation. So, we have basically 3 unknown labelled variable. Independent atomic species for this overall system we can clearly see that we have C and H. There is no non-reactive species involved the molecular species but we have one conversion relation that is known to us because the overall conversion is given in the problem statement.

So, that is one additional information that we can write, this gives the overall system degree of freedom by atomic species balance as zero. So, which means we can solve the overall system and that means these 3 unknowns are now known to us that n_6, n_7 and n_8. We will consider these are known now. So, when we apply it for separator the degree of freedom we will consider these are the known values.

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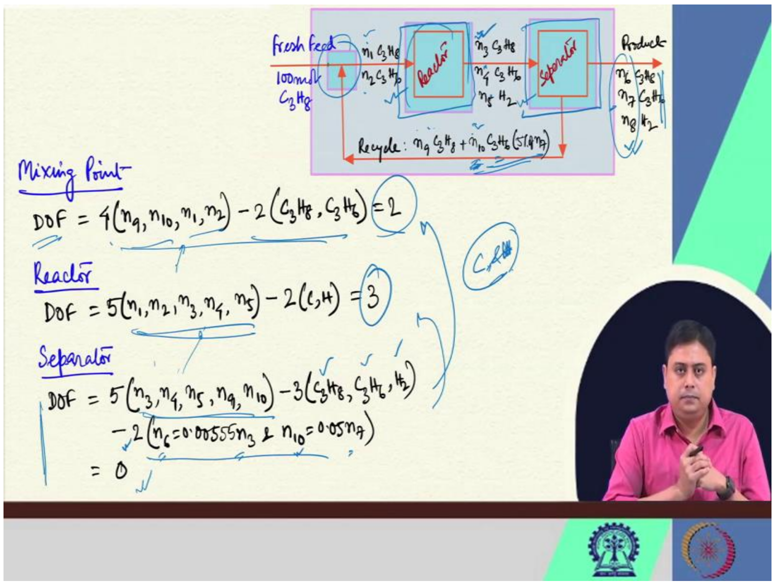

So now we go from say left to right, we come to the first mixing point degree of freedom analysis and then reactor and then we go for the separator what we have in the mixing point the degree of freedom analysis here in the mixing point it is the species that are mixed that are non-reactive. So, here we consider the molecular species balance that means the degree of freedom we identify for this mixing unit we have n_1, n_2, n_9 and n_{10} these are the things that are unknown – we have 2 independent molecular species that are mixed there C_3H_8 is mixed.

And we have another component C_3H_6. So, we can write 2 molecular species balance. So, the degree of freedom is 2 there. Now coming to the reactor, so, in the mixing point degree of freedom 2 means we cannot solve it with the present information. So, we move on to the next unit which is the reactor, in the reactor we identify that this is the system boundary in which we have n_1, n_2, n_3, n_4, n_5 this 5 are the unknowns the reactor reaction is happening.

So, as per the atomic species balance we have there only C and H these 2 atomic species we have on which we can write the balance there is no additional information provided there is no non-reactive molecular species. So, our degree of freedom in that case is 3. So, which means again the reactor cannot be solved independently or with the given information even after solving the overall system now we move on to the separator on the separator now you remember that we already calculated n_6, n_7, n_8 these are known to us.

So, for separator this subsystem the unknowns are n_3, n_4, n_5, n_9 and n_{10} we have 5 unknowns this is a separator a non-reactive part. So, we can do the molecular species balance the molecular species involved in separator we have 3, propane, propylene and hydrogen these are the 3 components. In addition to that we know 2 information's one is the relation between n_6 and n_3 that I explained in the last slide and the relation between n_7 and n_{10} that is the 5% relation.

And those relations n_6 is basically 0.555% of n_3 mentioned in the problem statement and n_{10} is 5% of n_7. So, which means we have 2 known information that means separator part can be solved easily. So, after overall system we must move to the separator the next stage or the sequence in which we will solve the problem. At first we will solve the overall system we will calculate these 3 unknown with the help of it we move to the separator and then again we go back to the other 2 system.

Because then once these 5 unknowns are known several of it are involved in the mixing and reactor and those can be solved by them.

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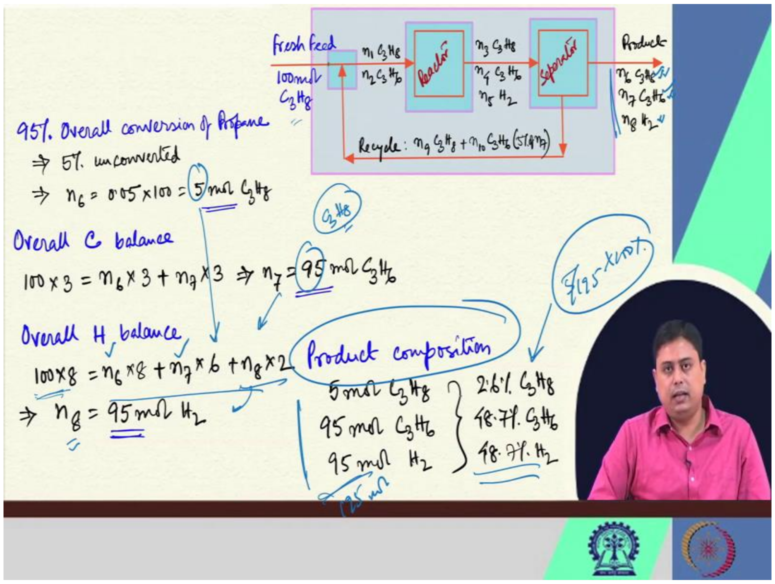

So, if we follow this strategy, first of all we have to deal with the given information we have to simplify it. It is said that it is 95% overall conversion is happening, 95% overall conversion of propane. So, which means we have 5% unconverted or unreacted that will leave the system the overall system which means n6 is basically 5% of the feed that is coming into the overall system 5% of 100 mole.

So, which mean n_6 is 5 mole, n_6 is known we have 2 unknowns for the overall process one is propylene and other one is hydrogen. So, now if we again look at the atomic carbon and atomic hydrogen balance because we have 2 species here. We can see here that n_6 is now known n_7 and n_8 these are 2 unknowns hydrogen is appearing in both the cases or with both of them whereas carbon is appearing in only one of them.

So, that is why it is logical that we write the overall carbon balance atomic carbon balance at first because it involves only one unknown which is n_7 in C_3H_8 one mole of propane involves 3 moles of atomic carbon. So, 100 × 3 and the output again n_6 × 3 it is the contribution from propane C_3H_8, n_7 is propylene it also has similar contribution C_3H_6. So, one mole of propylene involves 3 moles of atomic carbon and these summations of these 2 are the output which means we can easily calculate based on the n_6 value 5 mole that comes out to be n_7 as 95 mole.

And then we do the overall hydrogen balance. Now n_6 and n_7 both are known similar to our carbon balance input = output we have 100 × 8 because one mole of C_3H_8 contains 8 moles of atomic hydrogen and by that way we can understand that this is 100 × 8 = n_6 × 8, n_7 × 6 and n_8 × 2 summation of all the 3 terms in the output out of which we know n_6 and n_7.

So, n_8 we can easily calculate after substituting this 5 and 95 in this equation. So, which means we now know the product composition the product composition is 5 mole of C_3H_8, 95 moles of C_3H_6 and 95 moles of hydrogen we can easily find out what is the percentage molar percentage and the output composition or the product composition because this is 195 moles the total number of mole.

So, 5 divided by 195 × 100 would give us 2.6% and similarly the rest can be calculated. So, we know the output of the product composition we have to find out what is the recycle ratio.

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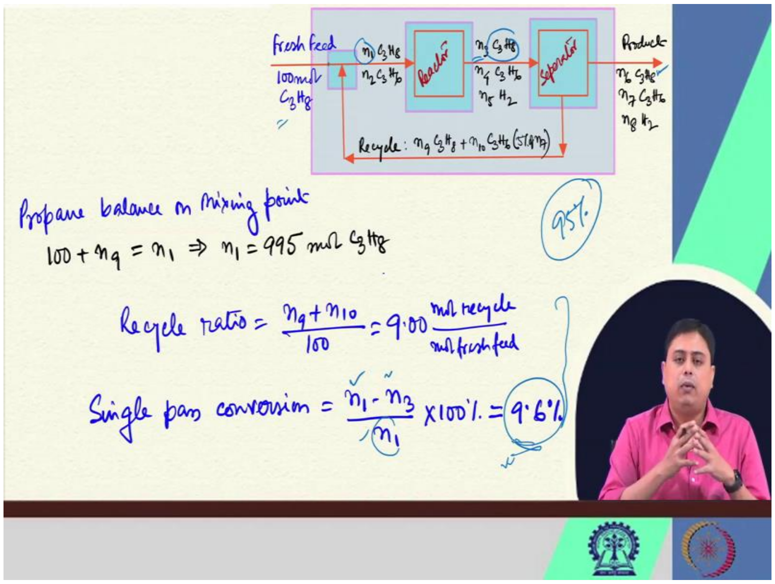

And the single pass conversion propane which means we have to find out n_3, n_1 and also we have to find out n_9, n_{10} etc. Now we know from these 2 given information n_6 and n_{10} because n_3 and n_6 are related by this expression we have calculated n_6. So, now n_3 is known to us n_3 is and n_6, n_6 is basically 0.555% of n_3. So, we can calculate what is the value of n_3 with the other additional information the relation between n_{10} and n_7 because n_7 is known.

So, we can calculate the value of n_{10} now we go to the separator because that was the sequence we decided and we have zero down based on the degree of freedom analysis, separator we can apply molecular species balance no reaction is happening there. So here if we apply propane balance around the separator or on the separator we see that n_3 is the input and the output is n_6 + n_9 simple balance n_6, n_3 is known. So, we find out the value of n_9.

So, n_9 and n_{10} both are known to us. So, similarly we can find out n_4 and n_5 from this balance by this simple molecular species balance that is input = output. So, which means n_4 and n_5 would be known to us if we apply propylene balance on the separator and hydrogen balance on the separator now if we apply. So, the remaining things are basically n_1, n_2 because these are now known, this set is known, this is also known only n_1 and n_2 are the things that are unknown to us.

So, for which if we now apply the propane balance on this mixing point it is the 100 mole of fresh feed + n_9 mole of propane that comes from the recycle = n_1 that goes n_2 the reactor. n_9 we have calculated the propane balance on the separator. So, n_1 just a simple arithmetic, once n_1 is known to us what we can calculate is basically that means now we have all the things that are known to us.

Similarly we can apply propylene balance on the mixing point and we can find out what is the value of n_2. So, the recycle ratio if it is asked and it has been asked in the problem statement the recycle ratio is nothing but the amount of recycle stream per mole of fresh feed that is here we have say n_9 + n_{10} these 2 values we have calculated. So, this is the recycle ratio which is around 9 moles of recycle per mole of fresh feed and the single pass conversions.

Because the overall conversion is known to us but what about the single pass conversion the efficiency of the reactor. The single pass conversion is nothing but if you identify clearly of propane the n_3 amount leaves the reactor n_1 amount is given to the feed. So, n_1 – n_3 that is reactant going to the reactor, reactant coming out from the reactor divided by the amount we are giving into the reactor.

If we substitute the numerics here we get that it is around 9.6% because all the values we have calculated previously. These are the questions that are asked in the problem statement along with the point that what are the unknowns I mean determine all the unknowns in the problem statement. So, what we see here is that the overall conversion was of 95% the single pass conversion is 9.6% which is say around 10% which means we have a very high efficiency separator that is placed after the reactor and it recycles most of the say 95% of the unconverted reactant back to the stream.

Because this n_6 came out to be 5 the base was 100 mole. So, this is the example of calculating single pass conversion and how it is different from the overall conversions. Because these things will be given in the problem statement say it would be mentioned this reactor has single pass conversion of 25% the overall conversion of the process is 98%. So, some this kind of information would be given and we have to extract the precise thing that we need while calculating or solving the problem.

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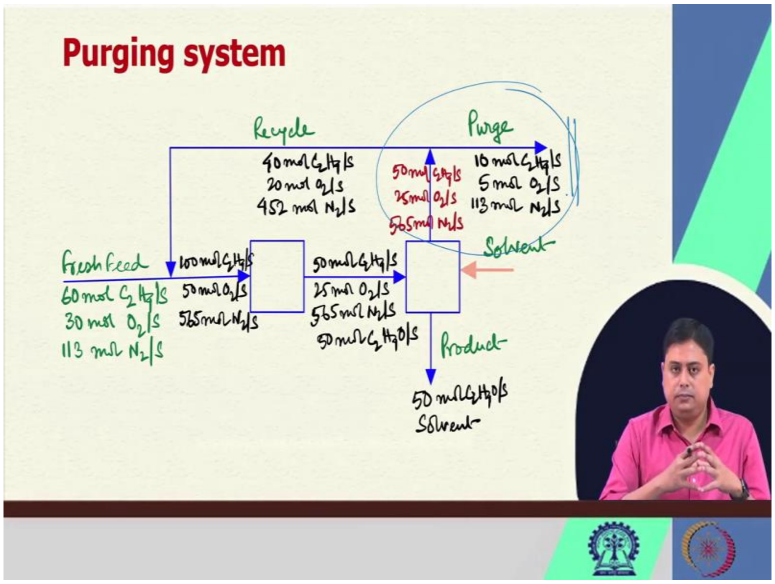

Now in addition to the recycle there will be necessity that we have some stream that we take out from the system as purge that is called the purging. It is necessary when we have recycle stream because say overall process something is being is reacted and some product is produced and there you have certain amount of inerts which is not taking part in the system and if there is a recycle stream like the point here it is shown.

What will happen that that inert will never escape the overall process and will continuously be in the loop and that will initiate the accumulation of that substance in the system and that may lead to some catastrophic failure. So, some portion of the recycle stream often is taken out from the system that is called purging of the system. So, for example here we have a fresh feed where nitrogen is inert.

Now if you follow this flow chart you would see that if the recycle stream is there without any purging stream the nitrogen will then start to accumulate in the system. But if we have a purge stream as a part or fraction from the recycle stream that is taken out from the product that chance is diminished. The thing that we must note and remember while labelling the flow chart is that the purge stream, the recycle stream and the stream from which these 2 streams are coming all these 3 points all the 3 streams will have the identical proportion of composition.

So, for example here if you see that from this branch from this stream we have purge and the recycle where we have 50 moles of ethylene 25 moles of oxygen and 656 mole of nitrogen. It is indeed that recycle + purge is this amount and at the same time it is of same composition in proportion.

That is here you have 1 : 2 in the ratio of oxygen and ethylene the same is here it is identical here if you multiply this stream the whole composition by a factor of 5 you actually get this composition. You multiply this with a factor of 4 you basically gets the recycle composition. So, which means these are same stream without any difference in composition it is just the mass balance you can write and eventually if 2 streams are known you can write the composition of the third stream easily.

It is simple the subtraction or it would be the addition if recycle and purge streams are known. So, this is another complicacy when you have multiple units with recycle. So, in those cases the purge stream will be like this and while labelling we have to be careful that there would be no composition change except the overall balance. From the overall balance you can write the components or the values the moles of those components but the molar percentage in percentage those remains identical.

So, with this I will stop today and in the next class we will see a different set of problem that involves combustion which is one of the major aspects in chemical reactions. Combustion is very important, these are frequently encountered in several presses. We will see couple of terminology in combustion that are important in the problem statement and will solve one problem related to that. Till then, thank you for your attention.