Aspen Plus Simulation Software
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Lecture – 27
Production of Cumene

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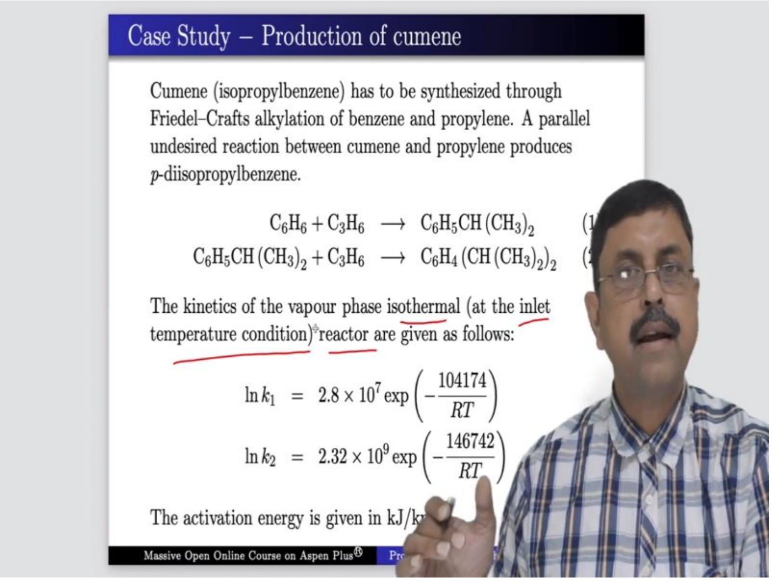

In today's lecture, we shall perform another case study that is on production of cumene. Cumene is actually another name for isopropylbenzene which can be synthesized through Friedel-Crafts alkylation reaction of benzene and propylene or propene. So, this is the main reaction and the desired reaction, reaction number 1 and the parallel undesired reaction between cumene and propylene produces p-diisopropylbenzene this one, this is undesired.

$$C_6H_6 + C_3H_6 \rightarrow C_6H_5CH(CH_3)_2 \quad \text{(desired equation)}$$

$$C_6H_5CH(CH_3)_2 + C_3H_6 \rightarrow C_6H_4(CH(CH_3)_2)_2 \quad \text{(undesired equation)}$$

So, this is the desired reaction, this is the undesired reaction. The kinetics of the vapour phase isothermal reactor are given as follows, here this is the activation energy which is given in kilo joule per kilo mole, these 2 things it is activation energy. So, this can be inserted at the proper place in aspen plus simulation window.

$$ln\ k_1 = 2.8 \times 10^7 \exp\left(-\frac{104174}{RT}\right)$$

$$\ln k_2 = 2.32 \times 10^9 exp\left(-\frac{146742}{RT}\right)$$

Now, the reactor is isothermal and it operates at the inlet temperature condition that means, whatever the temperature the feed material has the reactor operates at that temperature only.

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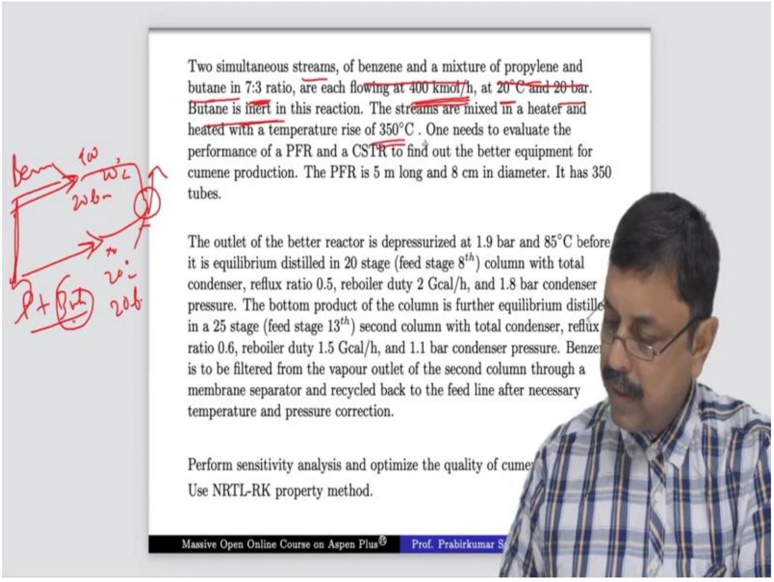
Two simultaneous streams, of benzene and a mixture of propylene and butane in 7:3 ratio, are each flowing at 400 kmol/h, at 20°C and 20 bar. Butane is inert in this reaction. The streams are mixed in a heater and heated with a temperature rise of 350°C . One needs to evaluate the performance of a PFR and a CSTR to find out the better equipment for cumene production. The PFR is 5 m long and 8 cm in diameter. It has 350 tubes.

The outlet of the better reactor is depressurized at 1.9 bar and 85°C before it is equilibrium distilled in 20 stage (feed stage 8^{th}) column with total condenser, reflux ratio 0.5, reboiler duty 2 Gcal/h, and 1.8 bar condenser pressure. The bottom product of the column is further equilibrium distille in a 25 stage (feed stage 13^{th}) second column with total condenser, reflux ratio 0.6, reboiler duty 1.5 Gcal/h, and 1.1 bar condenser pressure. Benze is to be filtered from the vapour outlet of the second column through a membrane separator and recycled back to the feed line after necessary temperature and pressure correction.

Perform sensitivity analysis and optimize the quality of cume
Use NRTL-RK property method.

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Some more information we have about the process, we have 2 simultaneous streams of benzene and a mixture of propylene and butane. So, we have one stream of benzene and another stream of propylene and Butane. Actually, benzene and propylene, they react with each other but butane is inert in this reaction. So, the mixture contains propylene and butane, in 7:3 ratios.

And both the streams they flow at 400 kmol/hr, 20 ℃ and 20 bar. So, both of them this is 400 this is 400. This is 20 ℃, this is also 20 ℃, this is 20 bar pressure this is also 20 bar pressure. And they are mixed into a heater and the temperature rise is 350 ℃.

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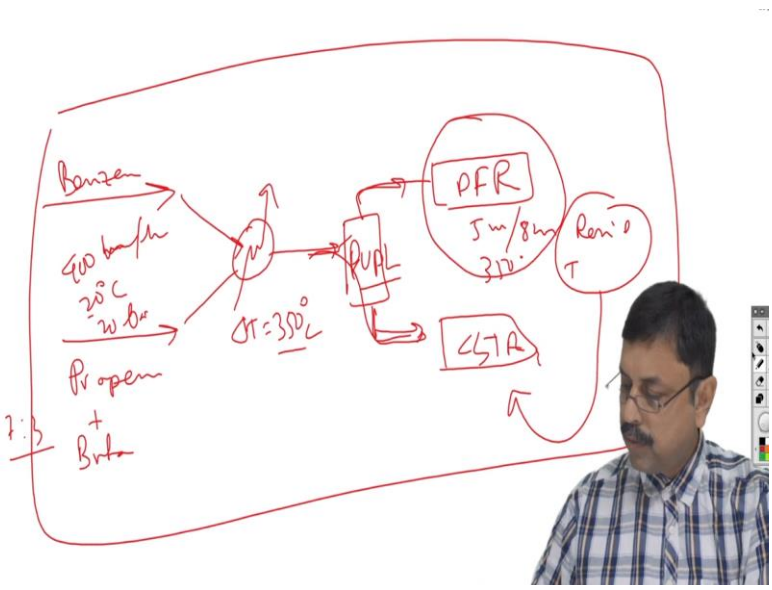

So, basically we have this benzene line, we have this propylene and butane line which is 7:3 ratios both of them are 400 kmol/hr 20 ℃ 20 bar pressure. They are mixed and heated where there is a temperature rise of 350 ℃. So, actually it becomes 350 + 20, so, 370 ℃ alone. Then one needs to evaluate the performance of PFR and CSTR to find out the better equipment for cumene production.

So, basically what we need to do, we need to employ a duplicator, duplicator means it duplicates the stream and the stream as well as, if 2 same stream is going in different direction. Here we will put a PFR and here we will put a CSTR and do the simulation and check the better equipment for cumene production. The PFL dimension has been given PFR is 5 m long and 8 cm in diameter it has 350 tubes.

So, this is 5 m length and 8 cm diameter 350 tubes. So, from this operation we will identify the residence time, we will identify the temperature, et cetera. That information will feed into the CSTR and then run both of them and check whichever is giving better production of cumene. And the subsequent run we will do on that particular reactor. So, first we will do up to this point and check which reactor performs better.

So, for that let us go to the simulation window and one more information that we have to remember we are supposed to use NRTL-RK property method. **(Video Starts: 06:03)** So, we have to add the components, first component is benzene then propene or propylene, same thing and they will produce cumene very common components so, it will identify as isopropanol benzene and butane there is the inert and the undesired product which is p-diisopropylbenzene.

So that we have to find diisopropylbenzene, I am not writing the whole thing whichever the component contains this name this part we will choose from there. Yes, this is the one which we are looking for p-diisopropylbenzene. So, we add this and we rename as p-diisopropylbenzene. Press next and we press NRTL-RK, press next run. Now, go to the simulation window so, we have to have one heater, one duplicator, one PFR. First let us use these 3 and the feed lines.

So, we have one heater, one duplicator and one PFR. So, this is our heater, this is our duplicator, this is the PFR. Let us change the icon this icon is not very good. So, this icon is good. Now, material in so, this is one material. It is benzene and this is the combination of propene and butane. This will go to the duplicator. So, duplicator will have one feed this will be PFROUT. Let us write here benzene or BENFEED and this one we can write other feed.

This one is MIXTURE, this one is PFRIN and this one is PFROUT. So, renaming is complete. Now, we have to give the components BENFEED input 20 ℃, 20 bar pressure and benzene molar flow rate is 400 kmol/hr. And then, other feed that is also 20 ℃, 20 bar pressure and molar flow rate 400 but they are in 7:3 ratios for propylene and butane.

So, this is mole fraction 0.7 and butane 0.3. So, we have 7:3 ratio of feed. Then we have to give the specification of heater which is temperature rise of 350 ℃. So, we do not write temperature over here, instead we will choose temperature change. So, we have a temperature rise of 350 ℃. There is no pressure drop in the line we will assume although it is not explicitly said in the statement.

But we will assume there is no pressure drop. And then, there is a duplicator nothing to fix over here and we have PFR. PFR we have to fix first reactor type, reactor with specified temperature and constant at inlet temperature. So that is what it has been said that isothermal reactor at the inlet temperature condition. So, it is inlet temperature condition configuration we have to check. What is the configuration? We have 5 m long and 8 cm diameter it has 350 tubes.

So, it is 5 m long diameter is 8 cm and it is a multitude reactor with 350 number of tubes and then we have to define the reactions. So, set the reaction which is a power law type and go to the reaction set mu, check the reactions. First is benzene plus propene produces cumene. So, it is benzene plus propene gives cumene. So, this is the one, this is the one, this is one, this exponent one, this exponent one, this exponent is 0.

Because actually the reaction is equal to k into concentration of benzene into concentration of propene is one only. So, we are not writing anything but concentration of cumene is 0. That means, this reaction rate does not depend upon the concentration of the product. So, we do not write any exponent over there. So, the first reaction is set and the second reaction is we have cumene plus propene is diisopropylbenzene.

So, it is cumene plus propylene is this one, here, also, –1, –1, 1, 1 and this is 1 exponential. So, we have to write kinetic properties it is a vapour phase reaction and the first reaction we have so,

$$ln\ k_1 = 2.8 \times 10^7 \exp\left(-\frac{104174}{RT}\right)$$

the k value is 2.8 is 7 and activation energy 104174 in kilo joule per kilo mole 104174 kJ/kmol and then secondary action again it is vapour phase

$$\ln k_2 = 2.32 \times 10^9 exp\left(-\frac{146742}{RT}\right)$$

k value is 2.32 10 to the power 9, and e = 146742 kilo joule per kilo mole.

So, reaction is set and the whole system is set. Now, run the system. So, just go to the PFR result. So, we have got a molar flow rate 69.933 kilo mole of cumene has been produced. And this much of unreacted benzene and propene are there butane remains unreactive as expected, because it is inert in this case. And a small amount of diisopropylbenzene also has been produced.

Check the results, we have 367.786 ℃. Now, one thing you should notice over here that we were sending the feed as 20 ℃ and they are coming to the heater. So, the heater outlet should be 20 ℃ and in the PFR we have asked for 350 ℃ delta T the temperature rise so, it should come at 370 ℃.

But here we find 367.786 slightly less than that why? Because of this mixing benzene and propene built in this combination they are getting mixed over here. So, the combined mixture is no longer at 20 ℃. It is coming below that and as a result with a temperature rise of 350 we are getting 367.786 ℃. This is the advantage of living certain calculations with as well it will provide more realistic picture, if it is allowed so.

So, we have this temperature, this is the heat duty you can write it in kilo watt or megawatt it is 1.9 megawatt heat duty and the residence time is only 16.6706 seconds. And the stream results already we know this is the stream results; these are the stream results we have got. Now, go to the main flow sheet we have to compare this with the performance of CSTR. So, bring in a CSTR over here and attach the lines.

So, rename them, this is CSTR in this is CSTR out and this is CSTR, keep it over here. And we have to fix the parameters of CSTR pressure again 0 pressure drop temperature. We have to fix temperature unfortunately; we do not have any means to give the temperature rise otherwise we could have given. So, we just write the exact temperature which we know it is 367.786 ℃; valid phases vapour only, specification type reaction volume.

But we do not have the information about the reaction volume over there as per the PFR combination but one thing is showed the PFR we know that residence time. So, what is the residence time of PFR it is 16.6706 seconds. So, the equivalent of residence time we will specify for CSTR also which is 16.6706. And the kinetics already you have set R 1 for PFR the same R 1 you can use for here and all is set.

Now, run the simulation. Now, you can just go and check the results. We can add in CSTR out over here. So that you can compare the PFR out and CSTR out side by side to check which one is better. So, temperature and pressure obviously, there is no change because you have said it and check the molar flow and mass flow. For PFR out we have got a cumene production of 69.933 kmol/hr whereas, through CSTR you get around 9 kmol/hr less.

So, we are at a disadvantageous position. So, the amount of benzene unreacted and propene unreacted is naturally it is higher in CSTR. So, in short we will not use the CSTR. So, the question that has been asked in the problem that is evaluates the performance of PFR and CSTR to find out the better equipment for cumene in production. So, without any doubt we can say that PFR is a better equipment for this purpose and we shall stick to it.

Now, we continue with the problem statement. So, the outlet of the better reactor. So, in this case it is PFR is depressurized at 1.9 bar and 85 ℃ before it is equilibrium distance. So, it is depressurizing so, it was operating at 20 bar pressure. So, we can use a valve for depressurization or directly we can depressurize into a heater or a cooler that will serve the purpose.

So, let us go over here so, place one exchanger, this is heater 2 and this is H2OUT and this one depressurized to 85 ℃ at 1.9 bar pressure. So, run it and we reach a value of it is showing 2 bar because actually we can set the display with 1 digit after a decimal point. So, it will show

1.9 bar pressure 85 ℃. What else? It is said it is equilibrium distilled in 20 stage column with total condenser reflux ratio re-boiler duty, all this information I have been given.

The bottom product of the column is further equilibrium distilled in another column there also the information has been given. So, basically we need to have 2 distillation columns 1 after another. So, the first column we use red flag. So, you connect this thing with this then 1 outlet, this outlet so, this one is column 1. what is H2 OUT? So, the stream results H2OUT you can check 329.872 kmol/hr of benzene.

This much of propane, this is cumene butane and some amount of DIPB. Now, here even without distillation, if you analyze the vapour liquid equilibrium of this components, you can very well understand that top product of the distillation column will mainly have benzene, propylene and butane. And the bottom product will mainly have cumene and P-DIPB.

So, these 2 will go mainly in the bottom and these 3 will go to the top even in the bottom product you may find some amount of benzene also. So, among benzene and cumene, benzene will go at the top and cumene will go at the bottom. Let us check the columns one by one. So, let us rename it as DIST and rename it as BOTT and we have to give the information about column one.

So, equilibrium based calculation, the number of stages we have 20 stages out of which feed stage is the 8th one. So, we have 20 stages, the fifth stage is the eighth one. The condenser will be total condenser and we have 2 informations over here re-boiler duty 2 GCal/hr and reflux ratio 0.5. So, 2 Giga calorie per hour reflux ratio 0.5. So, re-boiler duty 2 GCal/hr and reflux ratio 0.5.

And then pressure, I think the condenser pressure has been given 1.8 Bar condenser pressure. So, it is 1.8 bar of condensed pressure. Now, it is ready to run. So, run it and check the column results. Now, see the column result so, check the distillate. We have almost equal amount of benzene and propene in the distillate. Almost no cumene over there butane entire butane has gone to the distillate and almost no DIPB is there in the distillate.

Whereas, in the bottom line we have entire cumene, entire DIPB and considerable amount of benzene. So, cumene is the product, cumene is the main product in our system. So, we have to separate this cumene from benzene that is our goal. For that we need a second column for distillation. Through these distillations we expect cumene to be separated from benzene. So, let us attach a second column. So, press 1 second column over here, attach this, this is column 2.

Then this material out, and we will have mostly benzene over here and we will have cumene over here. So, we will just write these names. Let us check whether we can separate benzene and cumene in this manner. Now, obviously we have to give the parameters of column 2 which are available with us. So, go back to the problem statement we have 25 stages out of which 13 stages the feed stage.

So, we have 25 stages, the feed stream is 13th one, condenser is total condenser again the reboiler duty is 1.5 GCal/hr and reflux ratio 0.6. So, we have 1.5 GCal/hr and this is 0.6 pressure, 1.1 bar condenser pressure. So, we have 1.1 bar. Now, again we have set to run. So, the run is complete we can check the results of column 2 and the results are available over here, see the stream results.

So, you can check the cumene line, out of 68.4901, we have entirely cumene over here. Other things are very small amount. Benzene almost nil butane almost nil, propene and P-DIPB anyway they are not here in the cumene line but what about the benzene line, again benzene line will also have almost everything benzene except small quantity of cumene that is going through the benzene line and butane is almost nothing over here.

So, this is the difference between benzene line and cumene line. So, our target is to utilize this benzene because benzene we cannot throw. Cumene line is anyway this is our product. So, in the second column the cumene line is entirely cumene. So, this is our product but this benzene line we have to recycle. So, that we can use up this benzene.

For that we have this strategy with us. Benzene is to be filtered from the vapour outlet of the second column through a membrane separator and recycled back to the feed line after necessary temperature and pressure connection. So, what exactly we mean? We have this benzene line with us. So, this one we will pass through a membrane separator where benzene will be separated from all others.

And this benzene has to pass through some heater where temperature and pressure correction will be there and that we can attach with the feed line. So that this benzene can be reused in the system. So that is exactly what we are going to do in this line. So, further let us bring a separator. So, this is our separator and we bring a exchanger. So, this is our heater 3, this is our membrane separator.

And we will have one mixer because, we need a mixing line over here. So, this is a mixer, this line has to be fed into the membrane separator then the outlet of the membrane separator will go to this line, outlet of this we will go to this one. One more outlet we will go from here to here that will be purged. Then this one will be reconnected with a new destination which is this one and this line will be connected to this.

So, we have our full strategy in this manner, we can just write this. This name we can fix over here. So, we write it here as purge and this is the purified benzene. This is the recycles stream and this is the combined stream. We have to set the membrane separator where pure benzene will have 100% benzene and the purge line will automatically be set, heater will be used for pressure and temperature correction.

So that temperature has to be 367.786 °C, the pressure needs to be 20 bar. Now, we run the system once again so, recycling is complete, run it and we pray that it converges yes it is converged. So, the temperature and pressure of the recycle line is same as the feed line. And the pressure again we have to give extra digit after the decimal point otherwise we will not be able to understand it properly. It is 1.1 bar is the pressure.

So, the heater itself is working as a compressor and the heater, or else you can use a compressor and heater separately. So, it can be purged this way. Now, you check the cumene line one second cumene and benzene lines. So, go to the column 2, stream results. So that temperature of cumene line is 98.69. It is understandable because the bottom product is always at the higher temperature than the top product the molar fluids.

So, here we have a concert, you can check the cumene line. Earlier without recycling we had the cumene line with only cumene but now you find that along with cumene we have got extra 91.3034 kmol/hr of benzene that is coming along with the cumene line. And benzene line relatively gets free. It is 145.857. Earlier benzene line had benzene and some amount of cumene.

Now, benzene line is free of cumene, free of propene, free of other things also. So, earlier when there was no recycling then entire benzene was going through this line and enter cumene was going through this line. But now with the recycling on only that amount of benzene is being recycled in this loop which is useful and rest of the benzene which is coming into the system is having only one outlet that is over here.

So, this entire extra benzene is coming and coming out through this cumene line. In other words, this extra amount of benzene is not required in the system we can very well reduce the supply of benzene because unreacted Belgian is being recycled or why to supply extra benzene in the line. So, we want to reduce the benzene with an aim that we will increase the purity of cumene over here, as much as possible.

So, we will supply only that much of benzene into the system which is required. In other words, we shall vary benzene feed and check the purity of cumene. We have to optimize the supply of benzene. So, before optimization you can do certain sensitivity analysis. What it does? Sensitivity analysis means you can check for various benzene feed. What is the cumene purity? So, you can check cumene purity against the benzene flow rate.

So, for 200 kmol/hr benzene flow rate what is the cumene purity? For 300 kmol/hr what is the benzene purity? And so on. And try to find out where exactly your optimized purity may lie and then you can narrow down your range of optimization run. So, for that let us first take the help of the sensitivity analysis tool. So that will be obtained over here model analysis tools sensitivity, press new. Here you have to vary the benzene flow rate in the feed.

So, it is the type, mole flow of what benzene feed, component benzene. Now, ordinal flow is 400 kilometers per hour. So, let us check between 250 to 500 this wild guess, you can increase the range you can decrease the range also let us try between 250 and 500. And we will increment 10 kmol/hr. So, 250 then it will come 260, 270 et cetera. And then we will define 2 items, one is the cumene purity and also we will identify cumene flow rate.

What is cumene purity? Cumene purity is the mole fraction of cumene stream. What is the component? Component is cumene. And what is cume flow? Again it is mole flow, mole flow of cumene in the stream cumene. So, do not get confused between the name cumene everywhere. Here we are, we have given the name of the stream as cumene and here cumene is the component.

In the stream, this stream can be named anything q1, q2 anything. I have given the name cumene. So, got confused between the component and the stream. And go to tabulate, here you feel the variable of both Q and pure and then you can run the sensitivity analysis. So, it has successfully run just see the results and here you find the result. As expected at 400, your cumene flow rate is 69.9535 with the cumene purity of 0.43.

And as you increase the feed rate of benzene your cumene purity is going down and down. But look at the top. When you are sending very low flow rate your cumene purity is 1 that is 100% pure. But in the bargain your flow rate decreases. So, up to 280 kmol/hr your purity of cumene is within the limit and your flow rate is 68.954. So, you can always argue that you do not want 100% pure cumene, 99.9% purity will be enough for you.

Then it will arrive somewhere between 282 to 290 where this much of purity of cumene will be obtained. For instance, if you go to the simulation window and check you can give the flow rate instead of 400 you give 280 kmol/hr. And there is no requirement of sensitivity analysis tool over here. So, just make it inactive, you do not want to do the sensitivity on this analysis, so, run.

So, when you run and check the results once again, you can check the column output, yes. So, now we will check you have got almost entire cumene with very less amount of benzene and very less amount of butane and almost nothing is there. So, your cumene is absolutely pure over here. And benzene line obviously it will have the most which will be purified and in the bargain even losing 1.01 kmol/hr of cumene through the purge.

Because this benzene line is passed through the membrane separation unit and pure benzene is being sent over here rest of the thing is passed. So, cumene is being passed over here. So, you are losing 1.01168 kmol/hr of cumene through purge. But rest you can obtain. So, without losing the quality of cumene, you can get the best output of benzene. And we do not have to do any optimization over here.

Because the sensitivity analysis itself will tell you where we need to stop. So, we have performed the sensitivity analysis and optimize the quality of cumene production. So, with that we come to the end of this lecture and this case study. So, in the next lecture we will come with another interesting case study. Till then, Thank you and Goodbye.